



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:09 AM UTC

PDB ID : 5OIK / pdb_00005oik
EMDB ID : EMD-3817
Title : Structure of an RNA polymerase II-DSIF transcription elongation complex
Authors : Bernecky, C.; Plitzko, J.M.; Cramer, P.
Deposited on : 2017-07-18
Resolution : 3.70 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

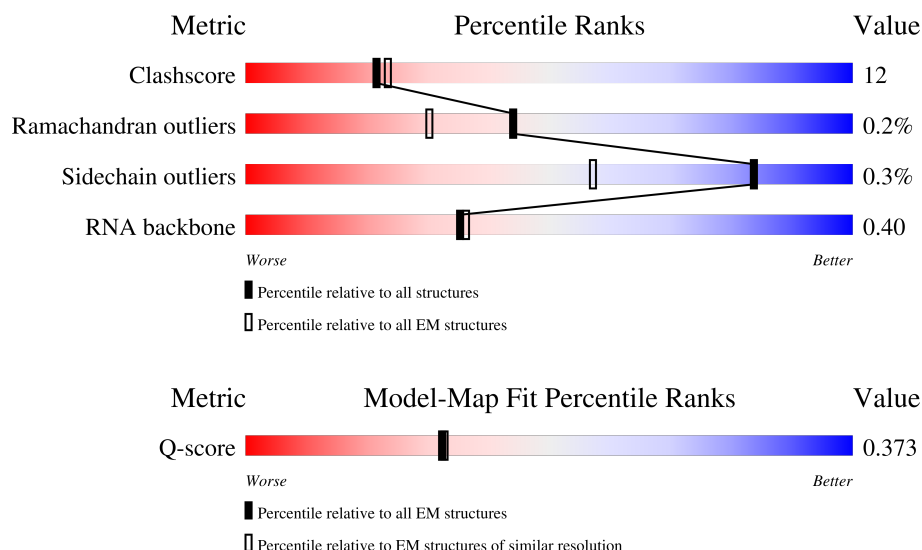
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11569 (3.20 - 4.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1970	
2	B	1174	
3	C	275	

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Mol	Chain	Length	Quality of chain
4	D	142	
5	E	210	
6	F	127	
7	G	172	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	N	43	
14	P	50	
15	T	43	
16	Y	117	
17	Z	1087	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 37988 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1421	Total	C	N	O	S	0	0
			11261	7084	2015	2090	72		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1147	Total	C	N	O	S	0	0
			9142	5780	1612	1686	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	259	Total	C	N	O	S	0	0
			2079	1305	357	411	6		

- Molecule 4 is a protein called Polymerase (RNA) II (DNA directed) polypeptide D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	128	Total	C	N	O	S	0	0
			1008	635	170	199	4		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1711	1084	300	319	8		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	82	Total	C	N	O	S	0	0
			658	419	113	121	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1341	871	218	244	8		

- Molecule 8 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	117	Total	C	N	O	S	0	0
			946	584	169	182	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			379	236	73	64	6		

- Molecule 13 is a DNA chain called DNA (43-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	43	Total	C	N	O	P	0	9
			709	335	130	202	42		

- Molecule 14 is a RNA chain called RNA (5'-R(P*UP*AP*UP*AP*UP*AP*CP*AP*UP*A

P*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	20	Total	C	N	O	P	0	0
			427	192	80	135	20		

- Molecule 15 is a DNA chain called DNA (43-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	43	Total	C	N	O	P	0	0
			874	419	157	256	42		

- Molecule 16 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	116	Total	C	N	O	S	0	0
			911	570	159	173	9		

- Molecule 17 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Z	488	Total	C	N	O	S	0	0
			3894	2475	686	716	17		

- Molecule 18 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
18	A	2	Total	Zn	0
			2	2	
18	B	1	Total	Zn	0
			1	1	
18	I	2	Total	Zn	0
			2	2	
18	J	1	Total	Zn	0
			1	1	
18	L	1	Total	Zn	0
			1	1	
18	Y	1	Total	Zn	0
			1	1	

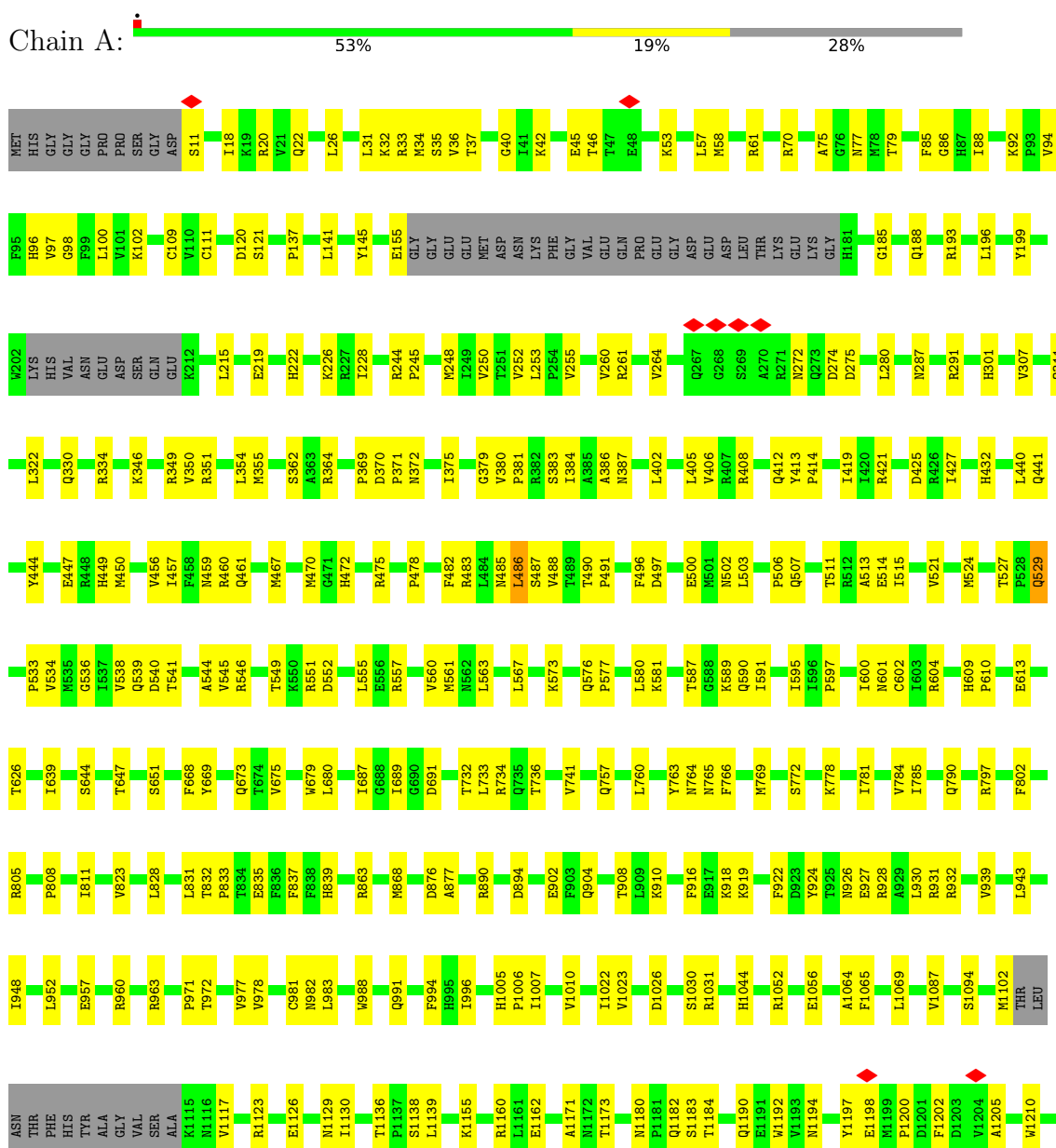
- Molecule 19 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

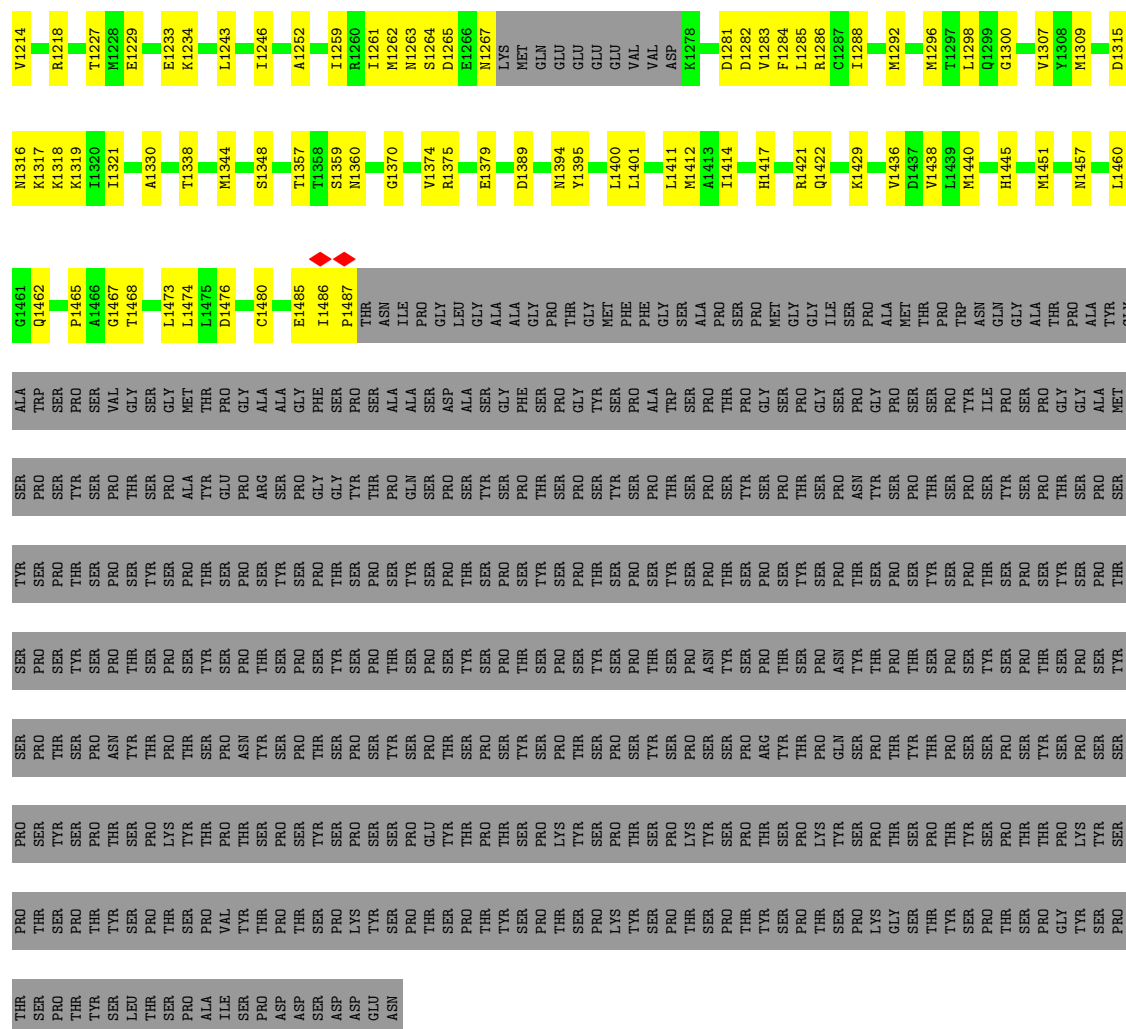
Mol	Chain	Residues	Atoms		AltConf
19	A	1	Total	Mg	0
			1	1	

3 Residue-property plots

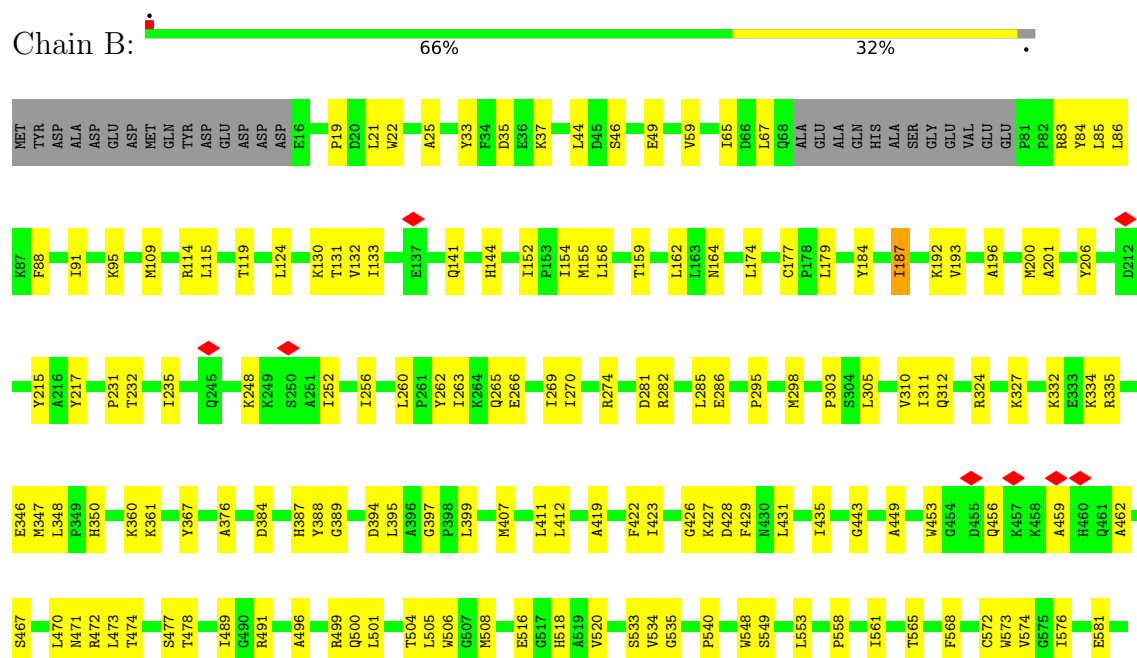
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

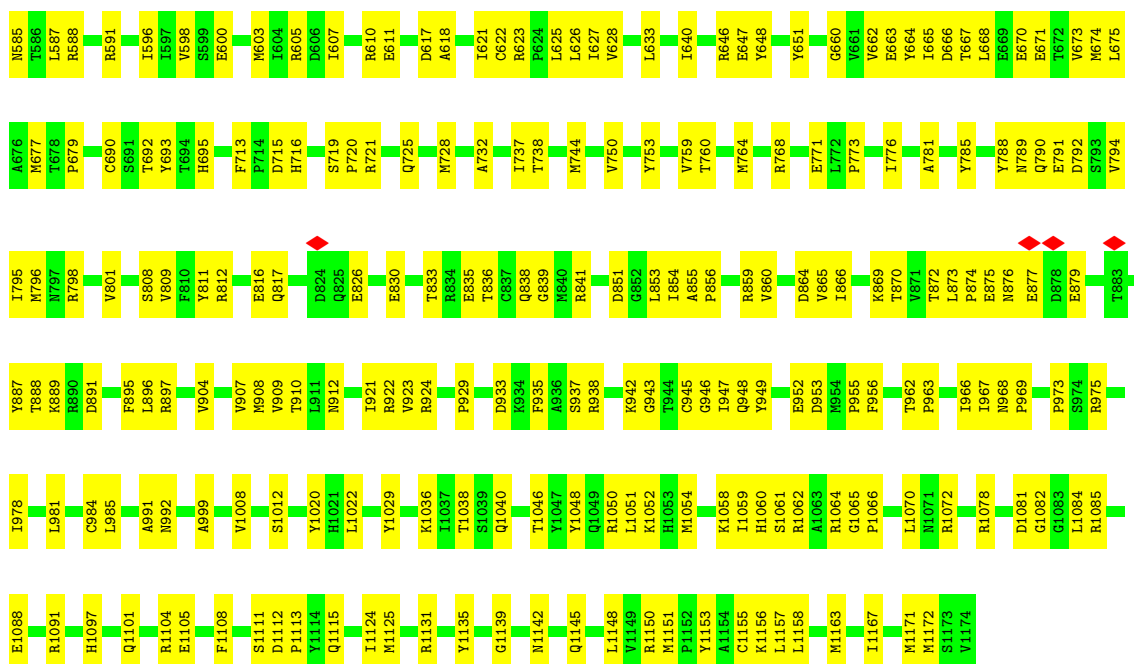
• Molecule 1: DNA-directed RNA polymerase II subunit RPB1





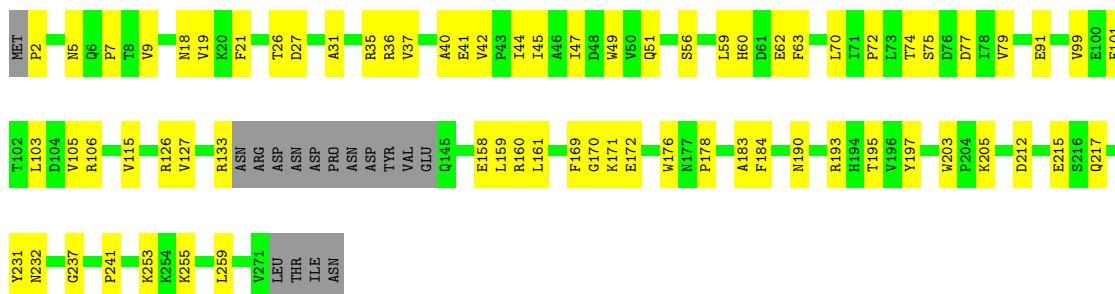
- Molecule 2: DNA-directed RNA polymerase subunit beta





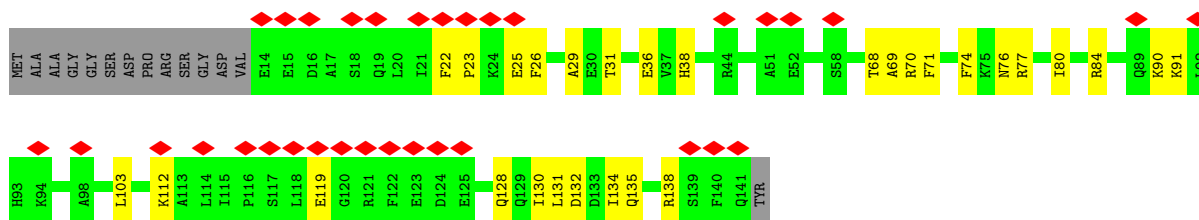
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 69% 25% 6%



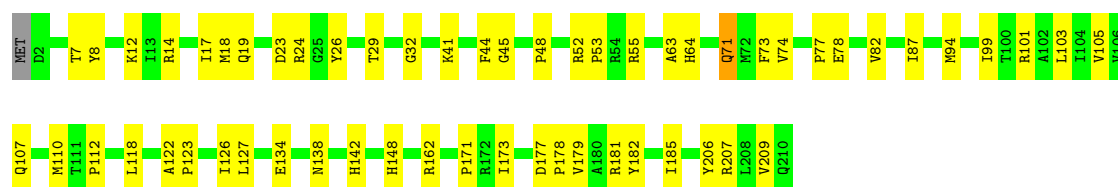
• Molecule 4: Polymerase (RNA) II (DNA directed) polypeptide D

Chain D: 23% 70% 20% 10%

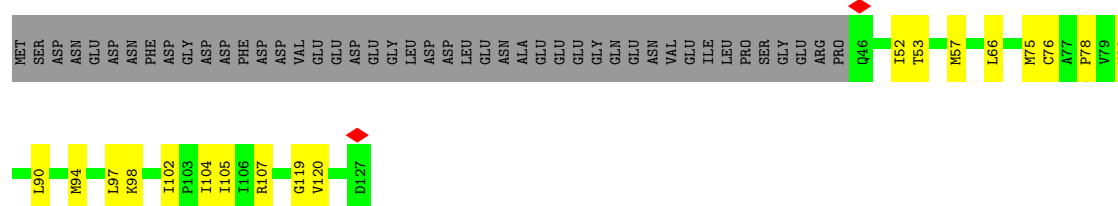


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

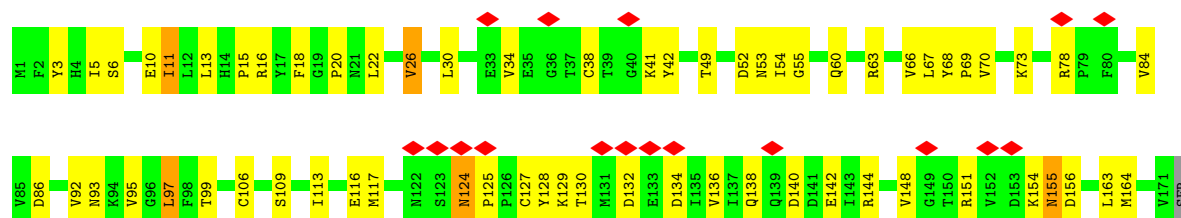
Chain E: 72% 27%



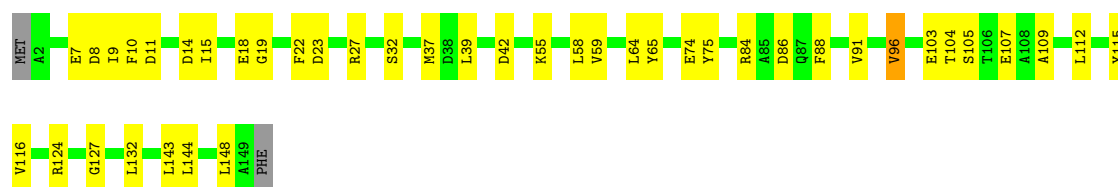
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



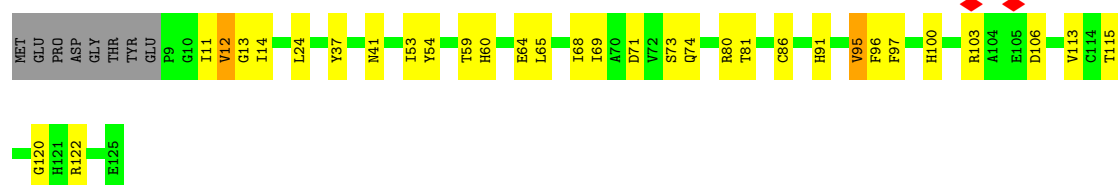
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



- Molecule 8: Uncharacterized protein



- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

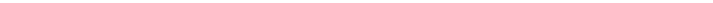


- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

M1	I2	P4	V5	R6			T9		I13		W18		Y21			T30		D33		L38		Y43			M48			H52	V53	D54	L55	I56			L60			L65	K66	E67
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- Chain K: 79% 19%

M1	N2	F10	K18	I19	T20	I21	C31	E38	T41	L42	I45	P54	P64	H65	P66	L67	E68	I72	F87	I91	I95	R104	F105	I109	G115	I1E	G1U
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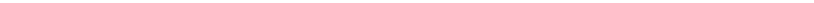
- Chain L:  47% 31% 22%

ME1	ASP	THR	GLN	LYS	ASP	VAL	GLN	PRO	PRO	LYS	GLN	GLN	P14	M15	I16	Y17		HP3		E27	I28	K29		I34	R35	C36	R37	C38	C39	G40	Y41	R42	I43	R44	M44	Y45	K46	R47	R48		V54		R58
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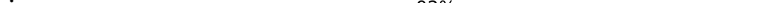
- Chain N: 

- Chain P:

U A A A C G C G A U C C U U A U U U G G C C A A C A A U U U U31 A32 U33 A34 U35 A36 C37 A38 U39 A40 A41 A42 C50

- Chain T:  5% 72% 26%

Category	Count
G1	1
T9	1
G21	1
C22	1
C23	1
T24	1
T29	1
A30	1
T31	1
A32	1
A35	1
A38	1
G41	1
C42	2
C43	2

- Chain Y:  35% 92% 6%

[illegible]

Chain Z:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	101140	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	33	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	37037	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.153	Depositor
Minimum map value	-0.053	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	345.6, 345.6, 345.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.47	0/11467	0.57	1/15479 (0.0%)
2	B	0.52	0/9325	0.61	0/12589
3	C	0.56	0/2122	0.60	0/2883
4	D	0.20	0/1022	0.60	0/1377
5	E	0.42	0/1742	0.56	1/2353 (0.0%)
6	F	0.48	0/668	0.59	0/903
7	G	0.26	0/1372	0.75	0/1861
8	H	0.50	0/1207	0.56	0/1628
9	I	0.35	0/968	0.57	0/1311
10	J	0.60	0/542	0.62	0/730
11	K	0.51	0/939	0.55	0/1271
12	L	0.49	0/385	0.57	0/511
13	N	0.30	0/785	0.80	0/1209
14	P	0.31	0/478	0.39	0/742
15	T	0.41	0/979	0.78	1/1508 (0.1%)
16	Y	0.73	1/927 (0.1%)	0.84	2/1250 (0.2%)
17	Z	0.80	2/3963 (0.1%)	0.91	14/5339 (0.3%)
All	All	0.52	3/38891 (0.0%)	0.65	19/52944 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
16	Y	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Y	105	GLY	CA-C	12.40	1.69	1.51
17	Z	450	ILE	CA-C	-6.40	1.45	1.52
17	Z	449	THR	CA-C	-6.09	1.46	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	104	ARG	N-CA-C	12.77	128.35	113.15
17	Z	449	THR	N-CA-C	-12.44	94.49	111.28
17	Z	450	ILE	N-CA-C	-11.05	94.18	109.21
17	Z	423	GLY	N-CA-C	10.35	127.01	114.69
17	Z	447	LYS	N-CA-C	-8.80	96.48	109.15
17	Z	268	LYS	N-CA-C	8.03	121.50	108.41
17	Z	396	PHE	CA-CB-CG	-6.47	107.33	113.80
17	Z	271	ALA	N-CA-C	6.45	118.02	108.60
17	Z	448	ILE	N-CA-C	-6.05	104.61	110.72
15	T	30	DA	C2'-C3'-O3'	-5.99	102.51	111.50
16	Y	106	VAL	N-CA-C	5.93	116.40	107.80
17	Z	267	VAL	CA-C-N	-5.89	114.70	123.00
17	Z	267	VAL	C-N-CA	-5.89	114.70	123.00
17	Z	286	TYR	CA-CB-CG	-5.85	103.36	113.90
5	E	71	GLN	CB-CA-C	-5.85	108.82	115.79
17	Z	423	GLY	CA-C-N	5.53	130.57	121.39
17	Z	423	GLY	C-N-CA	5.53	130.57	121.39
17	Z	363	GLY	N-CA-C	-5.32	107.45	115.32
1	A	486	LEU	CA-CB-CG	-5.06	98.60	116.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	910	LYS	Peptide
16	Y	105	GLY	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11261	0	11390	318	0
2	B	9142	0	9157	300	0
3	C	2079	0	2032	64	0
4	D	1008	0	970	20	0
5	E	1711	0	1733	42	0
6	F	658	0	686	18	0
7	G	1341	0	1348	47	0
8	H	1186	0	1147	36	0
9	I	946	0	881	26	0
10	J	533	0	553	15	0
11	K	920	0	942	19	0
12	L	379	0	386	17	0
13	N	709	0	387	11	0
14	P	427	0	216	10	0
15	T	874	0	487	14	0
16	Y	911	0	904	5	0
17	Z	3894	0	3957	87	0
18	A	2	0	0	0	0
18	B	1	0	0	0	0
18	I	2	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
18	Y	1	0	0	0	0
19	A	1	0	0	0	0
All	All	37988	0	37176	877	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (877) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:LYS:NZ	17:Z:250:TRP:CE3	2.09	1.20
17:Z:417:GLU:OE2	17:Z:516:ARG:NH1	1.84	1.08
17:Z:471:TYR:O	17:Z:472:PHE:CG	2.23	0.90
2:B:888:THR:HG23	2:B:889:LYS:HG3	1.56	0.88
1:A:425:ASP:HB2	17:Z:583:PHE:CZ	2.08	0.87
8:H:58:LEU:HD11	8:H:143:LEU:HD11	1.56	0.86
4:D:26:PHE:CE2	7:G:78:ARG:HD3	2.10	0.85
2:B:260:LEU:HD22	2:B:347:MET:HE1	1.58	0.85
7:G:60:GLN:OE1	7:G:63:ARG:NH2	2.09	0.85
17:Z:538:GLU:HG3	17:Z:577:ARG:HH22	1.44	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:45:GLY:HA3	5:E:52:ARG:HD2	1.60	0.83
15:T:29:DT:H2"	15:T:30:DA:OP1	1.77	0.83
14:P:37:C:OP2	17:Z:579:LYS:NZ	2.12	0.82
17:Z:479:LYS:HD3	17:Z:521:CYS:HB2	1.62	0.82
1:A:948:ILE:HG23	1:A:1007:ILE:HD11	1.61	0.82
17:Z:496:GLU:HB2	17:Z:499:PHE:HB2	1.62	0.80
1:A:425:ASP:CG	17:Z:583:PHE:CZ	2.60	0.80
1:A:425:ASP:OD2	17:Z:583:PHE:CZ	2.35	0.80
7:G:55:GLY:HA3	7:G:69:PRO:HG2	1.64	0.79
1:A:733:LEU:HB3	9:I:106:ASP:HB2	1.67	0.77
3:C:259:LEU:HD11	11:K:42:LEU:HD21	1.65	0.77
2:B:265:GLN:HE21	2:B:324:ARG:HE	1.31	0.77
1:A:372:ASN:ND2	2:B:788:TYR:OH	2.17	0.77
2:B:910:THR:HG22	12:L:43:ILE:HA	1.67	0.77
1:A:691:ASP:OD2	1:A:765:ASN:ND2	2.16	0.76
1:A:904:GLN:NE2	1:A:981:CYS:O	2.19	0.76
2:B:924:ARG:NH1	3:C:62:GLU:OE2	2.15	0.76
1:A:425:ASP:OD2	17:Z:583:PHE:CE1	2.39	0.76
2:B:591:ARG:NH2	2:B:663:GLU:OE2	2.18	0.76
2:B:841:ARG:HD2	2:B:895:PHE:HE2	1.51	0.76
17:Z:272:ASN:OD1	17:Z:384:GLU:HB2	1.85	0.76
1:A:447:GLU:OE1	2:B:1064:ARG:NH2	2.19	0.75
2:B:984:CYS:HG	2:B:1046:THR:HG1	1.25	0.75
1:A:538:VAL:HG12	1:A:539:GLN:HG2	1.68	0.75
17:Z:471:TYR:O	17:Z:472:PHE:CD2	2.40	0.74
9:I:65:LEU:O	9:I:122:ARG:NH1	2.15	0.74
9:I:86:CYS:HB3	9:I:91:HIS:H	1.53	0.74
1:A:425:ASP:CB	17:Z:583:PHE:CZ	2.71	0.74
2:B:568:PHE:HE1	2:B:573:TRP:HD1	1.35	0.74
2:B:367:TYR:OH	2:B:611:GLU:OE2	2.04	0.73
1:A:18:ILE:H	1:A:1462:GLN:HE22	1.36	0.73
2:B:851:ASP:OD2	12:L:17:TYR:OH	2.06	0.73
1:A:1374:VAL:HG11	1:A:1411:LEU:HD21	1.71	0.73
2:B:327:LYS:NZ	17:Z:250:TRP:CZ3	2.57	0.73
2:B:953:ASP:OD1	3:C:36:ARG:NH2	2.21	0.72
5:E:55:ARG:HB2	5:E:78:GLU:HG2	1.70	0.72
7:G:10:GLU:HB3	7:G:67:LEU:HG	1.71	0.72
5:E:185:ILE:HG21	5:E:209:VAL:HG21	1.72	0.72
2:B:193:VAL:HG21	2:B:470:LEU:HD13	1.72	0.72
5:E:19:GLN:OE1	5:E:138:ASN:ND2	2.22	0.72
4:D:26:PHE:HE2	7:G:78:ARG:HD3	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:984:CYS:SG	2:B:1046:THR:OG1	2.42	0.71
2:B:581:GLU:OE2	9:I:74:GLN:NE2	2.22	0.71
1:A:467:MET:SD	1:A:524:MET:HE2	2.30	0.71
4:D:70:ARG:NH2	7:G:140:ASP:OD1	2.23	0.71
2:B:37:LYS:NZ	2:B:664:TYR:OH	2.22	0.71
1:A:1192:TRP:HZ3	1:A:1246:ILE:HG22	1.56	0.71
1:A:863:ARG:NH2	1:A:1129:ASN:OD1	2.24	0.70
6:F:75:MET:O	7:G:15:PRO:HB2	1.91	0.70
3:C:2:PRO:HB3	11:K:54:PRO:HD2	1.73	0.70
1:A:413:TYR:OH	1:A:450:MET:O	2.10	0.70
1:A:1138:SER:OG	1:A:1360:ASN:ND2	2.25	0.70
2:B:759:VAL:HG12	2:B:999:ALA:HB2	1.74	0.70
3:C:42:VAL:HB	3:C:178:PRO:HG3	1.74	0.69
10:J:65:LEU:O	12:L:23:HIS:ND1	2.25	0.69
1:A:244:ARG:HD2	1:A:245:PRO:HD2	1.74	0.69
2:B:471:ASN:ND2	2:B:477:SER:OG	2.24	0.69
5:E:29:THR:HG23	5:E:32:GLY:H	1.56	0.69
1:A:577:PRO:HG2	1:A:580:LEU:HD23	1.75	0.69
2:B:565:THR:HA	2:B:610:ARG:HG2	1.75	0.68
2:B:1062:ARG:NH1	2:B:1081:ASP:O	2.26	0.68
2:B:360:LYS:HG2	2:B:553:LEU:HD13	1.75	0.68
1:A:877:ALA:HB3	1:A:890:ARG:NH1	2.09	0.68
7:G:97:LEU:HD13	7:G:113:ILE:HD11	1.76	0.68
1:A:597:PRO:HD3	1:A:668:PHE:CD1	2.28	0.68
2:B:781:ALA:HB3	2:B:966:ILE:HG12	1.76	0.68
1:A:760:LEU:HD22	1:A:764:ASN:HD22	1.59	0.68
1:A:540:ASP:HB2	2:B:790:GLN:HE21	1.59	0.67
1:A:877:ALA:HB3	1:A:890:ARG:HH11	1.59	0.67
1:A:757:GLN:HE22	1:A:778:LYS:HB3	1.59	0.67
1:A:1184:THR:HG21	1:A:1190:GLN:HA	1.77	0.67
2:B:327:LYS:NZ	17:Z:250:TRP:CD2	2.63	0.67
2:B:1029:TYR:CE1	2:B:1036:LYS:HG2	2.30	0.67
2:B:833:THR:HB	2:B:836:THR:HG22	1.76	0.67
9:I:115:THR:HG22	9:I:116:ALA:H	1.60	0.67
1:A:70:ARG:NH1	17:Z:535:GLU:OE2	2.28	0.67
1:A:560:VAL:HG22	1:A:591:ILE:HD11	1.77	0.67
2:B:270:ILE:HG13	2:B:305:LEU:HD23	1.76	0.66
7:G:164:MET:HE2	17:Z:494:ARG:HH12	1.60	0.66
1:A:760:LEU:HD22	1:A:764:ASN:ND2	2.11	0.66
1:A:111:CYS:SG	1:A:188:GLN:NE2	2.68	0.66
1:A:459:ASN:OD1	1:A:460:ARG:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:69:ILE:HG22	9:I:71:ASP:H	1.59	0.66
2:B:860:VAL:HG23	2:B:896:LEU:HD11	1.77	0.65
2:B:310:VAL:HG23	2:B:311:ILE:HD12	1.77	0.65
5:E:17:ILE:HD13	5:E:74:VAL:HG11	1.77	0.65
3:C:7:PRO:O	11:K:104:ARG:NH1	2.28	0.65
2:B:992:ASN:HD21	2:B:1020:TYR:HE2	1.44	0.65
1:A:425:ASP:HB2	17:Z:583:PHE:HZ	1.60	0.65
17:Z:479:LYS:NZ	17:Z:521:CYS:O	2.30	0.65
4:D:31:THR:HG22	7:G:3:TYR:HE1	1.62	0.64
5:E:73:PHE:HE2	5:E:99:ILE:HG12	1.61	0.64
1:A:425:ASP:OD2	17:Z:583:PHE:CE2	2.49	0.64
2:B:937:SER:HB3	2:B:1048:TYR:HE1	1.61	0.64
8:H:14:ASP:OD1	8:H:15:ILE:N	2.30	0.64
2:B:1085:ARG:HD3	15:T:22:DC:H5"	1.80	0.64
2:B:489:ILE:HD11	13:N:25:DA:C6	2.32	0.64
3:C:205:LYS:NZ	3:C:212:ASP:O	2.31	0.64
17:Z:703:ASN:OD1	17:Z:704:GLU:N	2.31	0.64
1:A:904:GLN:HE21	1:A:982:ASN:HA	1.63	0.64
1:A:1030:SER:HG	5:E:162:ARG:HE	1.42	0.64
1:A:402:LEU:HD23	1:A:405:LEU:HD12	1.80	0.64
1:A:1218:ARG:NH2	1:A:1252:ALA:O	2.31	0.64
3:C:31:ALA:O	3:C:231:TYR:OH	2.16	0.64
2:B:937:SER:HB3	2:B:1048:TYR:CE1	2.34	0.63
2:B:1062:ARG:NH2	2:B:1066:PRO:O	2.30	0.63
2:B:65:ILE:HB	2:B:86:LEU:HB2	1.80	0.63
2:B:952:GLU:OE2	3:C:40:ALA:HB2	1.98	0.63
5:E:55:ARG:NH1	5:E:107:GLN:HE21	1.97	0.63
15:T:30:DA:H2'	15:T:31:DT:C6	2.33	0.63
2:B:690:CYS:SG	2:B:692:THR:OG1	2.56	0.63
2:B:956:PHE:CE2	3:C:184:PHE:HB3	2.34	0.63
1:A:370:ASP:CG	11:K:65:HIS:HE2	2.07	0.62
1:A:1348:SER:O	5:E:12:LYS:NZ	2.32	0.62
2:B:907:VAL:HG22	2:B:921:ILE:HG12	1.81	0.62
3:C:105:VAL:HG11	3:C:115:VAL:HG22	1.79	0.62
1:A:1457:ASN:HD22	1:A:1465:PRO:HD3	1.64	0.62
8:H:64:LEU:HB3	8:H:84:ARG:HB2	1.79	0.62
17:Z:479:LYS:HG3	17:Z:489:THR:HG22	1.81	0.62
2:B:274:ARG:NH2	2:B:281:ASP:OD1	2.29	0.62
1:A:486:LEU:HD13	2:B:790:GLN:OE1	2.00	0.62
1:A:364:ARG:NH1	1:A:502:ASN:OD1	2.33	0.62
1:A:507:GLN:HB2	2:B:1105:GLU:OE2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:802:PHE:HE2	1:A:808:PRO:HD3	1.64	0.62
13:N:13:DA:C2	15:T:32:DA:C2	2.88	0.62
1:A:1202:PHE:O	1:A:1263:ASN:ND2	2.33	0.62
1:A:478:PRO:O	1:A:483:ARG:NH2	2.32	0.61
17:Z:469:ARG:HD2	17:Z:515:PRO:CG	2.30	0.61
1:A:957:GLU:HG2	1:A:960:ARG:HH21	1.64	0.61
5:E:52:ARG:HG3	5:E:53:PRO:HD3	1.80	0.61
3:C:99:VAL:HG21	3:C:127:VAL:HG21	1.81	0.61
1:A:45:GLU:OE2	1:A:53:LYS:NZ	2.34	0.61
1:A:1474:LEU:HB2	6:F:105:ILE:HG13	1.82	0.61
2:B:1060:HIS:NE2	2:B:1082:GLY:O	2.24	0.61
1:A:595:ILE:HD11	1:A:675:VAL:HG21	1.83	0.61
17:Z:267:VAL:O	17:Z:268:LYS:HD3	2.01	0.61
2:B:785:TYR:CZ	2:B:955:PRO:HD3	2.36	0.60
2:B:826:GLU:H	2:B:872:THR:HG22	1.67	0.60
2:B:839:GLY:O	2:B:891:ASP:HB3	2.02	0.60
12:L:36:CYS:HB2	12:L:44:MET:HE1	1.84	0.60
1:A:540:ASP:HB2	2:B:790:GLN:NE2	2.17	0.60
1:A:1417:HIS:O	1:A:1421:ARG:HG2	2.02	0.59
3:C:70:LEU:HD22	10:J:6:ARG:HG3	1.84	0.59
11:K:65:HIS:HE1	11:K:67:LEU:HD12	1.66	0.59
17:Z:745:VAL:HG21	17:Z:750:LEU:HD21	1.85	0.59
1:A:369:PRO:HB3	1:A:486:LEU:HD21	1.84	0.59
1:A:811:ILE:HD11	2:B:690:CYS:HB2	1.82	0.59
2:B:841:ARG:HD2	2:B:895:PHE:CE2	2.34	0.59
2:B:628:VAL:HG22	2:B:633:LEU:HD23	1.84	0.59
7:G:117:MET:SD	7:G:130:THR:HG23	2.42	0.59
1:A:20:ARG:NH2	2:B:1172:MET:SD	2.75	0.59
1:A:687:ILE:HD13	1:A:766:PHE:HE1	1.67	0.59
3:C:72:PRO:HG3	10:J:13:ILE:HD11	1.84	0.59
17:Z:472:PHE:HE1	17:Z:520:LEU:HB2	1.67	0.59
1:A:541:THR:O	1:A:545:VAL:HG23	2.03	0.59
6:F:94:MET:HE3	6:F:98:LYS:HE3	1.85	0.59
1:A:576:GLN:HG3	1:A:577:PRO:HD2	1.85	0.59
1:A:919:LYS:O	1:A:1052:ARG:HD3	2.03	0.59
2:B:501:LEU:HD12	2:B:505:LEU:HD12	1.84	0.59
1:A:475:ARG:NH2	11:K:68:GLU:OE2	2.36	0.58
1:A:551:ARG:HH12	8:H:27:ARG:HH21	1.51	0.58
2:B:130:LYS:NZ	2:B:429:PHE:O	2.35	0.58
2:B:933:ASP:OD2	2:B:1050:ARG:NH2	2.36	0.58
7:G:53:ASN:OD1	7:G:54:ILE:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ASP:OD2	17:Z:583:PHE:CD1	2.55	0.58
1:A:908:THR:HG23	1:A:916:PHE:HE1	1.67	0.58
1:A:1123:ARG:NH1	1:A:1126:GLU:OE1	2.33	0.58
3:C:75:SER:HB3	3:C:79:VAL:HG21	1.84	0.58
5:E:101:ARG:HG2	5:E:126:ILE:HD11	1.84	0.58
3:C:133:ARG:NH2	3:C:237:GLY:O	2.36	0.58
1:A:904:GLN:NE2	1:A:982:ASN:HA	2.18	0.58
8:H:32:SER:HB3	8:H:37:MET:H	1.67	0.58
1:A:274:ASP:OD1	1:A:275:ASP:N	2.35	0.58
2:B:924:ARG:HH12	3:C:62:GLU:CD	2.09	0.58
5:E:26:TYR:HD1	5:E:64:HIS:HA	1.67	0.58
6:F:52:ILE:O	6:F:53:THR:HG23	2.03	0.58
2:B:67:LEU:HD21	2:B:423:ILE:HG13	1.86	0.58
5:E:112:PRO:HB3	15:T:9:DT:H5"	1.85	0.58
1:A:461:GLN:HE22	1:A:502:ASN:ND2	2.01	0.57
1:A:601:ASN:CG	1:A:988:TRP:HZ3	2.12	0.57
2:B:508:MET:SD	2:B:667:THR:HG23	2.43	0.57
2:B:864:ASP:OD1	17:Z:725:LYS:NZ	2.36	0.57
2:B:663:GLU:OE1	2:B:695:HIS:NE2	2.27	0.57
2:B:956:PHE:HE2	3:C:184:PHE:HB3	1.66	0.57
3:C:5:ASN:HD21	3:C:26:THR:HA	1.70	0.57
5:E:48:PRO:HA	5:E:53:PRO:HG2	1.87	0.57
5:E:118:LEU:HD22	5:E:127:LEU:HB2	1.86	0.57
1:A:387:ASN:ND2	2:B:1061:SER:OG	2.30	0.57
2:B:84:TYR:CE2	2:B:423:ILE:HD12	2.39	0.57
2:B:796:MET:HE2	2:B:945:CYS:SG	2.44	0.57
1:A:576:GLN:HE21	1:A:580:LEU:HD21	1.68	0.57
2:B:841:ARG:NH2	14:P:39:U:O2	2.38	0.57
1:A:381:PRO:HG2	1:A:384:ILE:HB	1.85	0.57
1:A:971:PRO:O	1:A:972:THR:OG1	2.15	0.57
1:A:1473:LEU:HD22	6:F:104:ILE:HG21	1.86	0.57
2:B:760:THR:OG1	2:B:764:MET:SD	2.62	0.57
1:A:11:SER:N	2:B:1135:TYR:OH	2.38	0.57
1:A:876:ASP:O	1:A:890:ARG:NH1	2.37	0.57
1:A:1281:ASP:O	1:A:1285:LEU:N	2.36	0.57
1:A:802:PHE:HE2	1:A:808:PRO:CD	2.18	0.57
2:B:875:GLU:O	2:B:879:GLU:N	2.34	0.57
2:B:1115:GLN:HB3	2:B:1148:LEU:HD11	1.86	0.57
3:C:74:THR:O	3:C:127:VAL:HG12	2.05	0.57
2:B:179:LEU:HD22	2:B:768:ARG:HD3	1.87	0.56
2:B:667:THR:O	2:B:670:GLU:N	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Z:507:THR:HG22	17:Z:633:GLY:HA3	1.87	0.56
1:A:346:LYS:NZ	15:T:21:DG:OP2	2.38	0.56
1:A:576:GLN:O	1:A:590:GLN:NE2	2.38	0.56
2:B:177:CYS:HG	2:B:738:THR:HG1	1.53	0.56
5:E:74:VAL:HG22	5:E:103:LEU:HD12	1.86	0.56
1:A:1262:MET:HE2	1:A:1264:SER:HB3	1.88	0.56
3:C:47:ILE:HD11	3:C:101:PHE:HD2	1.70	0.56
1:A:994:PHE:CE2	1:A:1064:ALA:HA	2.41	0.56
4:D:112:LYS:HB3	4:D:119:GLU:OE2	2.06	0.56
1:A:555:LEU:HD12	1:A:591:ILE:HD12	1.86	0.56
2:B:387:HIS:NE2	2:B:671:GLU:OE2	2.38	0.56
1:A:1262:MET:HG2	1:A:1265:ASP:H	1.71	0.56
5:E:73:PHE:CE2	5:E:99:ILE:HG12	2.40	0.56
2:B:193:VAL:O	2:B:467:SER:HA	2.05	0.56
2:B:968:ASN:OD1	2:B:969:PRO:HD2	2.06	0.56
2:B:19:PRO:C	2:B:21:LEU:H	2.15	0.55
2:B:585:ASN:OD1	2:B:588:ARG:NH2	2.39	0.55
1:A:137:PRO:HB2	1:A:1445:HIS:HB3	1.88	0.55
1:A:457:ILE:HD11	1:A:515:ILE:HG12	1.87	0.55
1:A:1087:VAL:HG12	1:A:1400:LEU:HD22	1.88	0.55
1:A:1476:ASP:HB2	6:F:105:ILE:HG23	1.88	0.55
7:G:116:GLU:O	7:G:130:THR:HA	2.04	0.55
1:A:805:ARG:NH2	2:B:673:VAL:O	2.25	0.55
1:A:92:LYS:HD3	1:A:307:VAL:HG21	1.89	0.55
2:B:217:TYR:OH	9:I:103:ARG:NH2	2.39	0.55
3:C:18:ASN:OD1	3:C:19:VAL:N	2.39	0.55
17:Z:471:TYR:C	17:Z:472:PHE:CG	2.85	0.55
7:G:6:SER:HG	7:G:73:LYS:HZ3	1.53	0.55
16:Y:25:ILE:HD11	16:Y:50:TYR:CZ	2.42	0.55
17:Z:448:ILE:O	17:Z:449:THR:OG1	2.23	0.55
2:B:109:MET:HE2	2:B:174:LEU:HD13	1.88	0.55
2:B:131:THR:HG22	2:B:141:GLN:HB3	1.88	0.55
2:B:876:ASN:OD1	2:B:877:GLU:N	2.40	0.55
7:G:30:LEU:HD22	7:G:70:VAL:HG11	1.88	0.55
1:A:92:LYS:NZ	1:A:219:GLU:OE2	2.30	0.55
1:A:644:SER:O	1:A:651:SER:HB2	2.07	0.55
1:A:1130:ILE:HD13	1:A:1411:LEU:HD22	1.89	0.55
2:B:95:LYS:HB3	2:B:162:LEU:HD21	1.88	0.55
2:B:419:ALA:O	2:B:423:ILE:HG12	2.07	0.55
2:B:427:LYS:HG3	2:B:428:ASP:H	1.71	0.55
8:H:88:PHE:CD2	8:H:144:LEU:HB3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:MET:O	2:B:1091:ARG:HD2	2.07	0.55
7:G:92:VAL:HG13	7:G:128:TYR:CE2	2.41	0.55
17:Z:552:ARG:HB3	17:Z:559:GLN:HB2	1.88	0.55
1:A:514:GLU:OE2	2:B:1101:GLN:HB2	2.07	0.55
1:A:890:ARG:HE	1:A:1023:VAL:HG22	1.72	0.55
8:H:91:VAL:HG22	8:H:144:LEU:HD23	1.89	0.55
2:B:114:ARG:NH2	2:B:184:TYR:OH	2.39	0.54
2:B:347:MET:O	2:B:361:LYS:NZ	2.33	0.54
2:B:773:PRO:HG2	10:J:53:VAL:HG21	1.88	0.54
7:G:124:ASN:CB	7:G:125:PRO:HD3	2.37	0.54
1:A:1117:VAL:HA	1:A:1136:THR:HG21	1.89	0.54
1:A:1480:CYS:HA	6:F:80:MET:HE1	1.88	0.54
3:C:193:ARG:HH12	3:C:217:GLN:CD	2.15	0.54
8:H:112:LEU:HB2	8:H:132:LEU:HD23	1.90	0.54
5:E:63:ALA:HA	5:E:71:GLN:HA	1.89	0.54
17:Z:498:ASN:O	17:Z:515:PRO:HD3	2.08	0.54
3:C:5:ASN:ND2	3:C:26:THR:HA	2.22	0.54
2:B:1112:ASP:OD1	2:B:1112:ASP:N	2.34	0.54
5:E:7:THR:HG21	5:E:41:LYS:HZ3	1.73	0.54
5:E:171:PRO:HB2	5:E:207:ARG:HD3	1.90	0.54
15:T:29:DT:C2'	15:T:30:DA:OP1	2.51	0.54
2:B:617:ASP:OD1	2:B:618:ALA:N	2.40	0.54
1:A:386:ALA:O	1:A:449:HIS:ND1	2.41	0.54
2:B:422:PHE:HE2	2:B:429:PHE:HA	1.73	0.54
3:C:190:ASN:ND2	3:C:195:THR:O	2.40	0.54
1:A:26:LEU:HD13	1:A:31:LEU:HD21	1.90	0.54
1:A:228:ILE:O	1:A:244:ARG:NH2	2.26	0.54
2:B:692:THR:HG21	9:I:80:ARG:HH12	1.73	0.54
1:A:155:GLU:HA	1:A:185:GLY:HA2	1.90	0.54
2:B:833:THR:HG22	2:B:835:GLU:H	1.73	0.54
17:Z:466:GLN:OE1	17:Z:466:GLN:N	2.38	0.54
17:Z:607:HIS:HB3	17:Z:610:ARG:HD2	1.90	0.54
1:A:1005:HIS:ND1	1:A:1006:PRO:HD2	2.23	0.53
1:A:1234:LYS:NZ	1:A:1298:LEU:O	2.24	0.53
2:B:811:TYR:CD1	2:B:924:ARG:HB3	2.43	0.53
8:H:96:VAL:HA	8:H:116:VAL:HA	1.89	0.53
1:A:97:VAL:HG21	1:A:322:LEU:HD11	1.90	0.53
1:A:375:ILE:HD11	1:A:669:TYR:CD1	2.43	0.53
1:A:1184:THR:OG1	1:A:1190:GLN:NE2	2.41	0.53
2:B:119:THR:HG23	2:B:187:ILE:HA	1.90	0.53
2:B:587:LEU:HB3	2:B:603:MET:SD	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:31:THR:HG22	7:G:3:TYR:CE1	2.43	0.53
1:A:601:ASN:CG	1:A:988:TRP:CZ3	2.86	0.53
2:B:192:LYS:NZ	2:B:449:ALA:O	2.41	0.53
2:B:298:MET:HE2	9:I:14:ILE:HG21	1.89	0.53
1:A:425:ASP:CG	17:Z:583:PHE:CE2	2.86	0.53
2:B:109:MET:CE	2:B:174:LEU:HD13	2.39	0.53
2:B:516:GLU:HA	2:B:520:VAL:HG22	1.91	0.53
17:Z:519:GLN:NE2	17:Z:521:CYS:SG	2.81	0.53
1:A:384:ILE:HD11	2:B:1059:ILE:HG13	1.91	0.53
1:A:1344:MET:HE2	5:E:134:GLU:HA	1.91	0.53
1:A:18:ILE:HD12	2:B:1171:MET:HB3	1.90	0.53
1:A:511:THR:HG21	2:B:1105:GLU:OE1	2.08	0.53
1:A:245:PRO:HA	1:A:248:MET:HE2	1.89	0.53
1:A:1205:ALA:HB1	1:A:1267:ASN:HB2	1.90	0.53
2:B:533:SER:HB2	2:B:600:GLU:HG3	1.91	0.53
2:B:816:GLU:OE2	2:B:869:LYS:NZ	2.34	0.53
2:B:865:VAL:HG22	2:B:895:PHE:CE1	2.44	0.53
3:C:59:LEU:HD13	3:C:63:PHE:CE2	2.43	0.53
1:A:863:ARG:NH2	1:A:1414:ILE:O	2.41	0.53
1:A:1370:GLY:HA2	5:E:177:ASP:OD1	2.09	0.53
1:A:1451:MET:HE1	1:A:1460:LEU:HD12	1.89	0.53
2:B:625:LEU:HD13	2:B:675:LEU:HD21	1.91	0.53
10:J:21:TYR:HB2	10:J:38:LEU:HD11	1.91	0.53
2:B:789:ASN:HB3	2:B:795:ILE:HG13	1.92	0.52
3:C:44:ILE:HD12	3:C:178:PRO:HA	1.91	0.52
1:A:1052:ARG:HE	1:A:1056:GLU:CD	2.17	0.52
2:B:334:LYS:NZ	17:Z:236:LYS:NZ	2.57	0.52
2:B:728:MET:SD	2:B:942:LYS:HD3	2.50	0.52
1:A:868:MET:HE3	1:A:1401:LEU:HD13	1.91	0.52
1:A:1030:SER:OG	5:E:162:ARG:NE	2.28	0.52
1:A:1171:ALA:HA	9:I:59:THR:HB	1.92	0.52
9:I:113:VAL:HG22	9:I:122:ARG:HG2	1.90	0.52
1:A:287:ASN:O	1:A:291:ARG:HG2	2.09	0.52
1:A:926:ASN:C	1:A:928:ARG:H	2.17	0.52
2:B:1115:GLN:HG2	2:B:1150:ARG:HD2	1.91	0.52
8:H:58:LEU:HD11	8:H:143:LEU:CD1	2.35	0.52
13:N:13:DA:H2"	13:N:14:DT:H71	1.91	0.52
1:A:20:ARG:NH1	1:A:22:GLN:OE1	2.43	0.52
3:C:35:ARG:HB3	3:C:231:TYR:HE2	1.74	0.52
2:B:109:MET:HE2	2:B:174:LEU:HD22	1.91	0.52
2:B:456:GLN:H	2:B:456:GLN:CD	2.16	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:796:MET:SD	2:B:935:PHE:HE2	2.33	0.52
7:G:109:SER:HB3	17:Z:493:VAL:HG11	1.90	0.52
3:C:40:ALA:O	3:C:170:GLY:N	2.38	0.52
5:E:14:ARG:O	5:E:18:MET:HG2	2.10	0.52
17:Z:488:ASP:OD1	17:Z:489:THR:N	2.42	0.52
1:A:413:TYR:HB3	1:A:414:PRO:HD3	1.92	0.52
1:A:1026:ASP:OD1	1:A:1031:ARG:NH2	2.42	0.52
2:B:873:LEU:HD12	2:B:874:PRO:HD2	1.92	0.52
4:D:71:PHE:CZ	7:G:142:GLU:HG2	2.45	0.52
11:K:64:PRO:HG3	11:K:72:ILE:HD12	1.92	0.52
14:P:33:U:H2'	14:P:34:A:H8	1.75	0.52
1:A:364:ARG:HB2	2:B:1084:LEU:HD11	1.92	0.51
6:F:57:MET:HE1	6:F:120:VAL:HG13	1.90	0.51
9:I:81:THR:HG23	9:I:96:PHE:HE2	1.74	0.51
2:B:59:VAL:HG21	2:B:91:ILE:HD12	1.90	0.51
3:C:41:GLU:OE2	3:C:255:LYS:NZ	2.27	0.51
1:A:199:TYR:HE1	1:A:215:LEU:HD23	1.74	0.51
1:A:1485:GLU:HB3	6:F:78:PRO:HB3	1.92	0.51
2:B:1142:ASN:HD21	2:B:1145:GLN:HG3	1.75	0.51
1:A:994:PHE:HE2	1:A:1064:ALA:HA	1.76	0.51
2:B:295:PRO:HG3	9:I:11:ILE:HG23	1.92	0.51
2:B:798:ARG:HB2	2:B:948:GLN:HB3	1.92	0.51
2:B:1072:ARG:O	2:B:1112:ASP:HB3	2.11	0.51
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.91	0.51
13:N:4:DA:C2	15:T:41:DG:N2	2.78	0.51
2:B:217:TYR:CE2	2:B:376:ALA:HA	2.45	0.51
2:B:423:ILE:O	2:B:426:GLY:N	2.38	0.51
7:G:22:LEU:O	7:G:26:VAL:HG23	2.11	0.51
9:I:64:GLU:O	9:I:68:ILE:HG12	2.10	0.51
1:A:46:THR:HG23	1:A:58:MET:HB3	1.93	0.51
1:A:222:HIS:CD2	1:A:226:LYS:HE3	2.46	0.51
1:A:828:LEU:HD11	2:B:1008:VAL:HG21	1.92	0.51
2:B:470:LEU:HD11	2:B:478:THR:HG23	1.92	0.51
2:B:534:VAL:N	2:B:600:GLU:OE2	2.44	0.51
1:A:383:SER:OG	11:K:2:ASN:ND2	2.35	0.51
8:H:18:GLU:HG3	8:H:19:GLY:H	1.75	0.51
1:A:1102:MET:HG2	1:A:1389:ASP:OD2	2.10	0.51
2:B:22:TRP:O	2:B:25:ALA:N	2.43	0.51
2:B:474:THR:OG1	2:B:732:ALA:O	2.29	0.51
2:B:1151:MET:SD	2:B:1171:MET:HE1	2.50	0.51
5:E:45:GLY:HA3	5:E:52:ARG:HH11	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Y:25:ILE:CD1	16:Y:50:TYR:CZ	2.93	0.50
2:B:231:PRO:O	2:B:232:THR:HG23	2.10	0.50
2:B:411:LEU:HD11	2:B:435:ILE:HG23	1.94	0.50
5:E:148:HIS:CE1	5:E:179:VAL:HG11	2.46	0.50
3:C:40:ALA:HB1	3:C:171:LYS:HG3	1.94	0.50
8:H:64:LEU:HD13	8:H:84:ARG:HD2	1.94	0.50
1:A:98:GLY:HA3	1:A:1440:MET:HE2	1.94	0.50
1:A:784:VAL:HG22	2:B:978:ILE:HD11	1.93	0.50
2:B:792:ASP:O	2:B:943:GLY:HA3	2.12	0.50
14:P:36:A:H4'	14:P:37:C:OP1	2.11	0.50
1:A:552:ASP:OD1	8:H:22:PHE:HB3	2.11	0.50
1:A:573:LYS:NZ	8:H:74:GLU:OE2	2.33	0.50
2:B:692:THR:CG2	9:I:80:ARG:HH12	2.25	0.50
8:H:7:GLU:HG2	8:H:59:VAL:HG22	1.93	0.50
1:A:421:ARG:HA	1:A:444:TYR:CD1	2.46	0.50
7:G:92:VAL:HG21	7:G:127:CYS:HA	1.94	0.50
1:A:918:LYS:O	1:A:1052:ARG:NH2	2.45	0.50
2:B:459:ALA:HA	2:B:462:ALA:HB3	1.93	0.50
2:B:473:LEU:HD21	2:B:1052:LYS:HD3	1.93	0.50
4:D:103:LEU:HD11	7:G:84:VAL:HB	1.94	0.50
1:A:425:ASP:OD2	17:Z:583:PHE:CD2	2.66	0.49
1:A:733:LEU:HA	1:A:736:THR:HG22	1.94	0.49
17:Z:471:TYR:O	17:Z:472:PHE:CD1	2.63	0.49
1:A:506:PRO:HG3	1:A:515:ILE:HD12	1.94	0.49
1:A:687:ILE:HD11	1:A:769:MET:SD	2.53	0.49
3:C:159:LEU:HD11	3:C:161:LEU:HD23	1.94	0.49
16:Y:60:ILE:CD1	17:Z:190:ARG:HG3	2.42	0.49
2:B:193:VAL:HG23	2:B:470:LEU:HB2	1.94	0.49
10:J:56:ILE:O	10:J:60:LEU:HG	2.13	0.49
1:A:908:THR:HG23	1:A:916:PHE:CE1	2.46	0.49
1:A:1292:MET:O	1:A:1296:MET:HG2	2.11	0.49
2:B:35:ASP:OD2	2:B:646:ARG:NH2	2.44	0.49
7:G:11:ILE:N	7:G:11:ILE:HD13	2.28	0.49
1:A:1139:LEU:HB3	1:A:1338:THR:OG1	2.12	0.49
2:B:144:HIS:ND1	2:B:431:LEU:HD12	2.27	0.49
2:B:713:PHE:HB3	2:B:716:HIS:HD2	1.77	0.49
1:A:1182:GLN:O	1:A:1190:GLN:NE2	2.29	0.49
1:A:1286:ARG:HH21	9:I:54:TYR:HB2	1.78	0.49
2:B:115:LEU:HB3	2:B:908:MET:HE1	1.93	0.49
6:F:97:LEU:HD13	6:F:102:ILE:HD12	1.95	0.49
1:A:1227:THR:HG22	1:A:1229:GLU:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:LEU:HB2	2:B:131:THR:OG1	2.12	0.49
3:C:56:SER:HB2	3:C:158:GLU:H	1.78	0.49
3:C:169:PHE:HE1	3:C:171:LYS:HD2	1.77	0.49
14:P:33:U:H2'	14:P:34:A:C8	2.47	0.49
17:Z:474:MET:HA	17:Z:492:ILE:HG13	1.94	0.49
4:D:135:GLN:HA	4:D:138:ARG:HD3	1.95	0.49
5:E:122:ALA:HB3	5:E:123:PRO:HD3	1.94	0.49
9:I:73:SER:HA	9:I:95:VAL:HG11	1.95	0.49
10:J:3:ILE:HG13	10:J:4:PRO:HD2	1.95	0.49
17:Z:266:VAL:CG1	17:Z:268:LYS:HE2	2.43	0.49
1:A:255:VAL:HG13	1:A:280:LEU:HD13	1.95	0.49
1:A:421:ARG:NE	1:A:427:ILE:HD11	2.27	0.49
1:A:769:MET:SD	2:B:973:PRO:HG3	2.53	0.49
1:A:1288:ILE:HG22	1:A:1292:MET:HE2	1.95	0.49
1:A:1319:LYS:HE2	1:A:1321:ILE:HD11	1.93	0.49
2:B:256:ILE:HG22	2:B:269:ILE:HG13	1.95	0.49
2:B:491:ARG:HB3	2:B:518:HIS:HD2	1.77	0.49
3:C:9:VAL:HG11	11:K:105:PHE:HD1	1.78	0.49
1:A:1210:TRP:HZ3	9:I:53:ILE:HD12	1.77	0.48
2:B:159:THR:HA	2:B:164:ASN:ND2	2.28	0.48
2:B:196:ALA:HB2	2:B:395:LEU:HD23	1.94	0.48
3:C:45:ILE:HG13	3:C:79:VAL:HG22	1.95	0.48
5:E:173:ILE:HG23	5:E:209:VAL:HG22	1.94	0.48
7:G:148:VAL:HG21	17:Z:474:MET:HE2	1.95	0.48
8:H:11:ASP:OD1	8:H:55:LYS:HG2	2.13	0.48
13:N:12:DT:H5''	17:Z:283:ARG:NH2	2.27	0.48
1:A:40:GLY:O	1:A:42:LYS:HG3	2.13	0.48
2:B:334:LYS:NZ	17:Z:236:LYS:HZ3	2.11	0.48
2:B:910:THR:HG21	12:L:43:ILE:HG12	1.95	0.48
2:B:1101:GLN:HA	2:B:1104:ARG:HG2	1.96	0.48
7:G:93:ASN:O	7:G:128:TYR:OH	2.24	0.48
1:A:524:MET:HE1	2:B:1097:HIS:HE1	1.78	0.48
1:A:757:GLN:NE2	1:A:778:LYS:HB3	2.27	0.48
1:A:833:PRO:CB	2:B:677:MET:HE2	2.43	0.48
8:H:115:TYR:HE1	8:H:124:ARG:HD3	1.77	0.48
9:I:97:PHE:HB2	9:I:100:HIS:HE2	1.78	0.48
11:K:87:PHE:CE2	11:K:91:ILE:HD11	2.48	0.48
1:A:497:ASP:OD1	1:A:497:ASP:N	2.46	0.48
1:A:514:GLU:OE2	1:A:1468:THR:HG21	2.12	0.48
1:A:732:THR:HG22	1:A:734:ARG:H	1.79	0.48
2:B:84:TYR:HE2	2:B:423:ILE:HG23	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:795:ILE:HG12	2:B:947:ILE:HG22	1.95	0.48
2:B:835:GLU:O	2:B:887:TYR:HE1	1.96	0.48
17:Z:471:TYR:CG	17:Z:472:PHE:N	2.81	0.48
17:Z:521:CYS:HB3	17:Z:523:GLU:OE1	2.14	0.48
1:A:349:ARG:NH2	2:B:1070:LEU:HD21	2.29	0.48
1:A:868:MET:HE2	1:A:1401:LEU:HA	1.94	0.48
2:B:384:ASP:HB3	2:B:387:HIS:HB2	1.95	0.48
2:B:598:VAL:HG12	2:B:600:GLU:H	1.79	0.48
10:J:5:VAL:HG12	10:J:6:ARG:HG2	1.96	0.48
1:A:470:MET:HG2	1:A:524:MET:SD	2.54	0.48
1:A:485:ASN:ND2	1:A:673:GLN:OE1	2.37	0.48
8:H:104:THR:OG1	8:H:107:GLU:OE2	2.31	0.48
17:Z:728:THR:OG1	17:Z:731:THR:N	2.47	0.48
3:C:47:ILE:HD11	3:C:101:PHE:CD2	2.49	0.48
1:A:100:LEU:HD21	1:A:193:ARG:HD2	1.95	0.48
1:A:472:HIS:CE1	1:A:521:VAL:HG21	2.49	0.48
1:A:602:CYS:SG	1:A:604:ARG:HG2	2.54	0.48
1:A:823:VAL:HG11	1:A:831:LEU:HD22	1.95	0.48
2:B:866:ILE:HD11	2:B:896:LEU:HG	1.95	0.48
2:B:907:VAL:HG13	2:B:921:ILE:HG12	1.96	0.48
1:A:533:PRO:O	1:A:647:THR:OG1	2.26	0.47
5:E:44:PHE:O	5:E:53:PRO:HD3	2.14	0.47
8:H:88:PHE:HD2	8:H:144:LEU:HD22	1.79	0.47
17:Z:471:TYR:C	17:Z:472:PHE:CD2	2.91	0.47
1:A:456:VAL:HG21	1:A:503:LEU:HD11	1.96	0.47
2:B:1104:ARG:O	2:B:1108:PHE:HB3	2.14	0.47
2:B:19:PRO:O	2:B:21:LEU:N	2.44	0.47
2:B:812:ARG:HH12	2:B:897:ARG:HE	1.62	0.47
2:B:835:GLU:O	2:B:887:TYR:CE1	2.66	0.47
7:G:95:VAL:HG11	17:Z:630:VAL:HG21	1.96	0.47
1:A:96:HIS:HB2	1:A:250:VAL:HG23	1.96	0.47
7:G:99:THR:OG1	7:G:106:CYS:O	2.25	0.47
17:Z:706:ILE:HD11	17:Z:727:ALA:H	1.79	0.47
1:A:351:ARG:HG3	2:B:1088:GLU:OE2	2.15	0.47
2:B:854:ILE:HG22	2:B:855:ALA:O	2.15	0.47
7:G:127:CYS:HB2	7:G:138:GLN:HB3	1.97	0.47
17:Z:503:PHE:HD1	17:Z:508:MET:O	1.98	0.47
2:B:427:LYS:HG3	2:B:428:ASP:N	2.30	0.47
3:C:77:ASP:HB2	3:C:126:ARG:HH21	1.79	0.47
1:A:350:VAL:O	1:A:355:MET:HG2	2.14	0.47
1:A:496:PHE:HD2	2:B:791:GLU:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:924:TYR:HA	1:A:930:LEU:HD11	1.96	0.47
1:A:1318:LYS:HE2	1:A:1330:ALA:HB1	1.96	0.47
2:B:399:LEU:HB3	2:B:453:TRP:CZ2	2.49	0.47
2:B:535:GLY:N	2:B:600:GLU:OE2	2.27	0.47
4:D:135:GLN:OE1	4:D:138:ARG:NH1	2.47	0.47
15:T:23:DC:H2''	15:T:24:DT:H5'	1.96	0.47
2:B:44:LEU:HD23	2:B:155:MET:SD	2.55	0.47
3:C:59:LEU:HD13	3:C:63:PHE:HE2	1.80	0.47
3:C:72:PRO:HG3	10:J:13:ILE:CD1	2.45	0.47
5:E:171:PRO:HD2	5:E:206:TYR:O	2.15	0.47
1:A:610:PRO:HG2	1:A:613:GLU:HB2	1.96	0.47
2:B:389:GLY:O	2:B:668:LEU:HD23	2.15	0.47
2:B:407:MET:HE3	2:B:443:GLY:HA3	1.96	0.47
13:N:4:DA:C2	15:T:41:DG:C2	3.03	0.47
17:Z:535:GLU:O	17:Z:538:GLU:HG2	2.14	0.47
1:A:406:VAL:HG11	1:A:419:ILE:HD11	1.97	0.47
1:A:457:ILE:HG13	1:A:515:ILE:HD13	1.97	0.47
1:A:460:ARG:NH2	14:P:50:C:O2'	2.42	0.46
1:A:524:MET:CE	2:B:1097:HIS:HE1	2.28	0.46
1:A:902:GLU:OE1	1:A:982:ASN:HB2	2.15	0.46
2:B:744:MET:HE1	2:B:922:ARG:HB2	1.97	0.46
1:A:379:GLY:O	1:A:482:PHE:HA	2.16	0.46
1:A:425:ASP:OD2	17:Z:583:PHE:CG	2.68	0.46
5:E:77:PRO:HD2	5:E:105:VAL:O	2.15	0.46
7:G:86:ASP:OD1	7:G:144:ARG:NE	2.48	0.46
1:A:1026:ASP:O	1:A:1031:ARG:NH1	2.48	0.46
1:A:408:ARG:HH21	1:A:412:GLN:HB3	1.79	0.46
1:A:587:THR:HG22	1:A:589:LYS:H	1.80	0.46
1:A:609:HIS:ND1	1:A:626:THR:OG1	2.31	0.46
1:A:760:LEU:HD11	1:A:781:ILE:HG21	1.97	0.46
1:A:839:HIS:CD2	2:B:719:SER:HB3	2.50	0.46
2:B:572:CYS:O	2:B:574:VAL:HG23	2.15	0.46
5:E:24:ARG:NH2	5:E:181:ARG:O	2.48	0.46
17:Z:447:LYS:HA	17:Z:464:PRO:HA	1.97	0.46
2:B:750:VAL:O	2:B:808:SER:HB2	2.16	0.46
8:H:103:GLU:HB3	8:H:109:ALA:HB2	1.96	0.46
1:A:301:HIS:HD2	17:Z:259:GLU:OE1	1.98	0.46
14:P:33:U:H4'	17:Z:619:ARG:HG2	1.97	0.46
17:Z:502:LEU:HD11	17:Z:511:LEU:HD12	1.98	0.46
1:A:527:THR:HB	1:A:534:VAL:CG2	2.45	0.46
1:A:557:ARG:O	1:A:561:MET:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:ALA:HB3	2:B:206:TYR:OH	2.16	0.46
2:B:812:ARG:HH12	2:B:897:ARG:NE	2.13	0.46
2:B:904:VAL:HG22	2:B:923:VAL:HG22	1.98	0.46
2:B:1151:MET:HE2	2:B:1156:LYS:N	2.31	0.46
5:E:94:MET:HG2	5:E:99:ILE:HD11	1.98	0.46
1:A:362:SER:HA	1:A:503:LEU:O	2.16	0.46
2:B:633:LEU:HD11	2:B:679:PRO:HG3	1.98	0.46
2:B:812:ARG:NH1	2:B:897:ARG:HE	2.13	0.46
2:B:854:ILE:CD1	2:B:866:ILE:HA	2.46	0.46
2:B:540:PRO:HB2	2:B:596:ILE:HG23	1.97	0.46
2:B:753:TYR:O	2:B:776:ILE:HG12	2.16	0.46
1:A:33:ARG:HB3	2:B:1139:GLY:HA2	1.98	0.46
1:A:597:PRO:HD3	1:A:668:PHE:HD1	1.78	0.46
1:A:802:PHE:HE1	2:B:504:THR:HG22	1.81	0.46
1:A:1394:ASN:OD1	1:A:1395:TYR:N	2.48	0.46
2:B:949:TYR:HB3	2:B:953:ASP:HB2	1.98	0.46
7:G:10:GLU:HB3	7:G:67:LEU:CG	2.43	0.46
1:A:37:THR:HG22	1:A:61:ARG:HD2	1.98	0.45
1:A:432:HIS:NE2	17:Z:728:THR:HG22	2.31	0.45
1:A:790:GLN:NE2	1:A:797:ARG:HG3	2.31	0.45
2:B:605:ARG:NH1	2:B:607:ILE:HG12	2.31	0.45
2:B:622:CYS:HB3	2:B:666:ASP:HB3	1.98	0.45
2:B:1062:ARG:NH1	2:B:1065:GLY:HA3	2.31	0.45
3:C:103:LEU:O	3:C:160:ARG:HA	2.17	0.45
6:F:105:ILE:HA	6:F:119:GLY:HA2	1.97	0.45
12:L:16:ILE:HG12	12:L:27:GLU:HG2	1.99	0.45
1:A:1451:MET:CE	1:A:1460:LEU:HD12	2.45	0.45
1:A:1467:GLY:O	1:A:1468:THR:HB	2.17	0.45
2:B:955:PRO:O	2:B:963:PRO:HD2	2.16	0.45
2:B:1029:TYR:CD1	2:B:1036:LYS:HG2	2.50	0.45
8:H:18:GLU:HG3	8:H:19:GLY:N	2.31	0.45
1:A:488:VAL:O	1:A:491:PRO:HD2	2.16	0.45
1:A:741:VAL:HG11	1:A:797:ARG:NH1	2.31	0.45
3:C:7:PRO:HB3	3:C:26:THR:OG1	2.17	0.45
3:C:259:LEU:HD22	11:K:19:ILE:HD11	1.98	0.45
17:Z:417:GLU:CD	17:Z:516:ARG:NH1	2.68	0.45
1:A:922:PHE:CD2	1:A:952:LEU:HD23	2.52	0.45
1:A:1375:ARG:HH12	1:A:1379:GLU:CD	2.25	0.45
2:B:856:PRO:HG2	12:L:48:ARG:HA	1.97	0.45
6:F:52:ILE:O	6:F:52:ILE:HG13	2.15	0.45
1:A:350:VAL:HA	1:A:354:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:SER:OG	1:A:673:GLN:NE2	2.49	0.45
2:B:388:TYR:CE2	2:B:621:ILE:HG21	2.52	0.45
2:B:627:ILE:HD12	2:B:660:GLY:O	2.16	0.45
2:B:715:ASP:OD1	2:B:715:ASP:N	2.47	0.45
3:C:77:ASP:OD2	3:C:126:ARG:NH2	2.50	0.45
5:E:82:VAL:HB	5:E:110:MET:SD	2.56	0.45
8:H:10:PHE:CE2	8:H:39:LEU:HD22	2.50	0.45
12:L:17:TYR:HE1	12:L:46:LYS:HD2	1.82	0.45
1:A:11:SER:N	2:B:1135:TYR:HH	2.14	0.45
1:A:375:ILE:HD11	1:A:669:TYR:CG	2.51	0.45
3:C:172:GLU:HG2	11:K:10:PHE:CE1	2.52	0.45
7:G:97:LEU:HD12	7:G:128:TYR:CE2	2.52	0.45
1:A:34:MET:HE1	2:B:1124:ILE:HD13	1.98	0.45
3:C:49:TRP:NE1	12:L:54:VAL:HG11	2.32	0.45
8:H:55:LYS:O	8:H:148:LEU:N	2.46	0.45
1:A:102:LYS:HZ1	1:A:141:LEU:HD13	1.82	0.45
1:A:932:ARG:NH2	8:H:103:GLU:OE1	2.45	0.45
1:A:1262:MET:HB3	1:A:1265:ASP:HB2	1.99	0.45
2:B:419:ALA:HA	2:B:429:PHE:CE1	2.52	0.45
2:B:548:TRP:O	2:B:549:SER:OG	2.24	0.45
3:C:197:TYR:HD2	3:C:217:GLN:HE21	1.64	0.45
7:G:129:LYS:CB	7:G:136:VAL:HG22	2.47	0.45
1:A:1065:PHE:CE2	1:A:1069:LEU:HD11	2.52	0.45
2:B:496:ALA:O	2:B:500:GLN:HG3	2.16	0.45
2:B:794:VAL:O	2:B:946:GLY:N	2.30	0.45
2:B:859:ARG:HD2	17:Z:737:HIS:HA	1.99	0.45
1:A:109:CYS:SG	1:A:145:TYR:HA	2.57	0.45
1:A:529:GLN:O	1:A:1394:ASN:HB2	2.17	0.45
1:A:922:PHE:H	1:A:1052:ARG:HD2	1.82	0.45
3:C:19:VAL:HG12	3:C:21:PHE:HD1	1.81	0.45
6:F:76:CYS:O	7:G:16:ARG:HA	2.18	0.45
7:G:92:VAL:HG13	7:G:128:TYR:CD2	2.52	0.45
11:K:21:ILE:HG23	11:K:31:CYS:SG	2.57	0.45
17:Z:509:HIS:HD2	17:Z:552:ARG:NH1	2.15	0.45
1:A:837:PHE:HB2	2:B:506:TRP:HZ3	1.81	0.44
2:B:350:HIS:HD2	2:B:572:CYS:SG	2.41	0.44
2:B:489:ILE:HD11	13:N:25:DA:C5	2.51	0.44
2:B:801:VAL:HG13	2:B:929:PRO:HG2	1.98	0.44
2:B:962:THR:O	10:J:9:THR:HG23	2.18	0.44
2:B:978:ILE:O	2:B:981:LEU:N	2.44	0.44
6:F:75:MET:HB2	7:G:15:PRO:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Z:224:TYR:HE2	17:Z:226:TYR:CZ	2.35	0.44
1:A:35:SER:OG	1:A:86:GLY:HA2	2.17	0.44
1:A:1197:TYR:HD1	1:A:1200:PRO:HB3	1.81	0.44
2:B:581:GLU:CD	9:I:74:GLN:HE22	2.22	0.44
2:B:1012:SER:HB3	2:B:1022:LEU:HB2	2.00	0.44
2:B:1124:ILE:HG22	2:B:1125:MET:N	2.31	0.44
1:A:983:LEU:HD23	1:A:983:LEU:HA	1.80	0.44
2:B:838:GLN:HB2	2:B:887:TYR:HB3	1.99	0.44
3:C:19:VAL:HG23	3:C:241:PRO:HB2	1.99	0.44
17:Z:482:ALA:HA	17:Z:486:GLU:OE1	2.17	0.44
17:Z:514:LEU:HB3	17:Z:515:PRO:HD2	1.99	0.44
1:A:461:GLN:HE22	1:A:502:ASN:HD21	1.66	0.44
1:A:549:THR:O	1:A:589:LYS:HE3	2.18	0.44
1:A:1173:THR:HG23	1:A:1214:VAL:HG12	1.99	0.44
2:B:568:PHE:HE1	2:B:573:TRP:CD1	2.25	0.44
2:B:991:ALA:HB1	10:J:43:TYR:HB2	1.99	0.44
8:H:37:MET:HG2	8:H:127:GLY:HA3	2.00	0.44
9:I:106:ASP:OD1	9:I:106:ASP:N	2.50	0.44
17:Z:484:ARG:HH11	17:Z:485:PHE:HE1	1.64	0.44
1:A:576:GLN:HA	8:H:75:TYR:HB2	1.98	0.44
2:B:1078:ARG:N	15:T:24:DT:OP1	2.51	0.44
7:G:132:ASP:C	7:G:134:ASP:H	2.25	0.44
17:Z:734:VAL:HG21	17:Z:750:LEU:HD21	1.99	0.44
1:A:441:GLN:HG2	1:A:444:TYR:CE2	2.52	0.44
2:B:809:VAL:HG21	3:C:60:HIS:CE1	2.52	0.44
2:B:260:LEU:CD2	2:B:347:MET:HE1	2.38	0.44
10:J:3:ILE:HD13	10:J:18:TRP:HB2	1.99	0.44
14:P:39:U:H2'	14:P:40:A:C8	2.52	0.44
1:A:581:LYS:NZ	8:H:86:ASP:O	2.50	0.44
1:A:1486:ILE:HG13	1:A:1487:PRO:HD3	1.99	0.44
2:B:533:SER:HB2	2:B:600:GLU:CG	2.47	0.44
9:I:24:LEU:HB3	9:I:37:TYR:HB3	1.98	0.44
1:A:551:ARG:NH1	8:H:42:ASP:OD2	2.51	0.44
1:A:802:PHE:CE1	2:B:504:THR:HG22	2.53	0.44
1:A:1243:LEU:HD11	1:A:1259:ILE:HG23	2.00	0.44
2:B:215:TYR:OH	2:B:266:GLU:OE2	2.27	0.44
2:B:262:TYR:CD2	2:B:346:GLU:HG3	2.53	0.44
4:D:36:GLU:CD	4:D:84:ARG:HH21	2.25	0.44
5:E:177:ASP:OD1	5:E:178:PRO:HD2	2.18	0.44
12:L:46:LYS:O	12:L:46:LYS:HG3	2.18	0.44
1:A:544:ALA:HB2	1:A:680:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1163:MET:HA	2:B:1167:ILE:O	2.18	0.43
17:Z:479:LYS:NZ	17:Z:523:GLU:O	2.31	0.43
1:A:371:PRO:HD2	2:B:788:TYR:CE2	2.52	0.43
1:A:1139:LEU:HD13	1:A:1359:SER:HB3	1.99	0.43
2:B:49:GLU:OE1	2:B:534:VAL:HG22	2.18	0.43
2:B:472:ARG:HD3	2:B:472:ARG:HA	1.82	0.43
10:J:48:MET:O	10:J:52:HIS:HB2	2.18	0.43
17:Z:469:ARG:HD2	17:Z:515:PRO:HG3	1.99	0.43
1:A:1436:VAL:O	1:A:1440:MET:HG2	2.19	0.43
2:B:285:LEU:HD23	2:B:298:MET:HE1	1.99	0.43
2:B:794:VAL:HG22	2:B:967:ILE:HG22	2.01	0.43
2:B:1155:CYS:O	2:B:1158:LEU:HB3	2.18	0.43
1:A:57:LEU:O	1:A:261:ARG:NH2	2.49	0.43
2:B:1111:SER:O	2:B:1113:PRO:HD3	2.18	0.43
3:C:212:ASP:OD1	3:C:215:GLU:HG2	2.19	0.43
7:G:38:CYS:HB3	7:G:155:ASN:O	2.19	0.43
10:J:30:THR:O	10:J:33:ASP:N	2.51	0.43
11:K:105:PHE:CE2	11:K:109:ILE:HD11	2.53	0.43
17:Z:492:ILE:HG13	17:Z:492:ILE:O	2.19	0.43
1:A:196:LEU:HD13	1:A:311:GLN:HG3	2.01	0.43
1:A:927:GLU:HG3	1:A:943:LEU:HD11	2.00	0.43
1:A:1229:GLU:O	1:A:1233:GLU:HG2	2.19	0.43
1:A:1284:PHE:CE2	1:A:1288:ILE:HD11	2.54	0.43
2:B:187:ILE:HG21	2:B:449:ALA:HB2	2.00	0.43
2:B:235:ILE:HG21	2:B:348:LEU:HD11	2.00	0.43
4:D:25:GLU:OE2	7:G:41:LYS:HE3	2.19	0.43
5:E:23:ASP:OD2	5:E:182:TYR:OH	2.32	0.43
17:Z:386:VAL:O	17:Z:387:LYS:HB2	2.18	0.43
1:A:760:LEU:HD21	1:A:785:ILE:CD1	2.48	0.43
1:A:1429:LYS:HB2	1:A:1438:VAL:HG11	2.01	0.43
2:B:1050:ARG:HH21	2:B:1054:MET:HG2	1.83	0.43
4:D:90:LYS:HE2	4:D:130:ILE:HD11	1.99	0.43
17:Z:469:ARG:HD2	17:Z:515:PRO:CB	2.49	0.43
1:A:354:LEU:HD21	2:B:1155:CYS:HA	2.00	0.43
1:A:540:ASP:CB	2:B:790:GLN:HE21	2.30	0.43
1:A:1162:GLU:O	1:A:1300:GLY:HA3	2.18	0.43
1:A:1316:ASN:OD1	1:A:1317:LYS:HG2	2.19	0.43
12:L:14:PRO:HG3	12:L:29:LYS:HB3	2.00	0.43
1:A:260:VAL:HG22	2:B:1157:LEU:HD12	2.01	0.43
2:B:558:PRO:O	2:B:561:ILE:HG22	2.19	0.43
9:I:60:HIS:O	9:I:60:HIS:ND1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Z:361:PHE:O	17:Z:362:GLU:C	2.62	0.43
2:B:561:ILE:HG13	2:B:576:ILE:HG21	2.00	0.43
2:B:647:GLU:O	2:B:648:TYR:CG	2.72	0.43
4:D:22:PHE:HB3	4:D:23:PRO:HD2	2.01	0.43
8:H:10:PHE:CE1	8:H:32:SER:HB2	2.53	0.43
17:Z:486:GLU:OE2	17:Z:555:ARG:NH2	2.52	0.43
1:A:597:PRO:HG2	1:A:600:ILE:HD12	2.00	0.42
2:B:332:LYS:O	2:B:335:ARG:N	2.49	0.42
1:A:36:VAL:HG22	1:A:85:PHE:O	2.19	0.42
1:A:500:GLU:OE2	2:B:1058:LYS:HB3	2.18	0.42
1:A:1139:LEU:HB3	1:A:1338:THR:HG1	1.84	0.42
2:B:719:SER:OG	2:B:720:PRO:HD3	2.20	0.42
3:C:40:ALA:O	3:C:169:PHE:HB2	2.19	0.42
16:Y:14:ARG:HD2	16:Y:25:ILE:HD12	2.01	0.42
1:A:764:ASN:OD1	1:A:765:ASN:N	2.52	0.42
1:A:823:VAL:HG13	1:A:835:GLU:HB3	2.01	0.42
1:A:1007:ILE:O	1:A:1010:VAL:N	2.51	0.42
1:A:1316:ASN:OD1	1:A:1317:LYS:N	2.52	0.42
1:A:1357:THR:O	5:E:142:HIS:NE2	2.50	0.42
1:A:1412:MET:SD	1:A:1422:GLN:NE2	2.92	0.42
2:B:428:ASP:OD1	2:B:429:PHE:N	2.47	0.42
2:B:1038:THR:HA	3:C:195:THR:HA	2.01	0.42
7:G:13:LEU:HD22	7:G:68:TYR:CE1	2.55	0.42
13:N:7:DA:C2	15:T:38:DA:C2	3.07	0.42
17:Z:271:ALA:O	17:Z:272:ASN:HB3	2.18	0.42
1:A:94:VAL:HG13	1:A:311:GLN:OE1	2.19	0.42
1:A:527:THR:HB	1:A:534:VAL:HG22	2.01	0.42
1:A:1474:LEU:HB2	6:F:105:ILE:CG1	2.48	0.42
11:K:18:LYS:NZ	11:K:38:GLU:OE2	2.40	0.42
12:L:39:CYS:SG	12:L:40:GLY:N	2.92	0.42
12:L:41:TYR:CE2	12:L:43:ILE:HB	2.55	0.42
2:B:84:TYR:CD1	2:B:132:VAL:HG12	2.55	0.42
2:B:499:ARG:NH1	2:B:520:VAL:O	2.50	0.42
3:C:253:LYS:HE3	11:K:95:ILE:HG23	2.02	0.42
5:E:8:TYR:CZ	5:E:12:LYS:HE3	2.54	0.42
15:T:30:DA:H2''	15:T:31:DT:H5'	2.02	0.42
1:A:991:GLN:HA	1:A:996:ILE:HD12	2.01	0.42
2:B:33:TYR:CE1	2:B:37:LYS:HD2	2.54	0.42
2:B:1072:ARG:NH1	2:B:1153:TYR:CZ	2.88	0.42
1:A:832:THR:HG1	1:A:835:GLU:CD	2.27	0.42
1:A:1282:ASP:OD1	1:A:1283:VAL:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:665:ILE:HD11	2:B:695:HIS:NE2	2.35	0.42
2:B:737:ILE:HD12	2:B:737:ILE:HG23	1.85	0.42
2:B:909:VAL:HG12	12:L:34:ILE:HD11	2.00	0.42
3:C:37:VAL:HG13	3:C:41:GLU:HB2	2.02	0.42
7:G:10:GLU:C	7:G:11:ILE:HD13	2.44	0.42
7:G:154:LYS:C	7:G:156:ASP:H	2.27	0.42
12:L:47:LYS:HG2	12:L:48:ARG:H	1.83	0.42
1:A:264:VAL:HB	1:A:272:ASN:HB2	2.00	0.42
1:A:490:THR:HB	1:A:491:PRO:HD3	2.02	0.42
1:A:977:VAL:HG12	1:A:978:VAL:N	2.35	0.42
2:B:548:TRP:O	2:B:548:TRP:CG	2.73	0.42
2:B:1040:GLN:HG2	3:C:203:TRP:CH2	2.55	0.42
3:C:49:TRP:CH2	3:C:51:GLN:HB2	2.54	0.42
8:H:10:PHE:HE1	8:H:32:SER:HB2	1.84	0.42
1:A:1194:ASN:O	1:A:1198:GLU:HG3	2.20	0.42
1:A:1315:ASP:HA	1:A:1318:LYS:HD3	2.00	0.42
3:C:91:GLU:OE2	17:Z:751:THR:HG21	2.19	0.42
3:C:106:ARG:NH1	3:C:158:GLU:OE1	2.53	0.42
3:C:172:GLU:OE1	3:C:176:TRP:CZ3	2.73	0.42
4:D:29:ALA:HB2	7:G:5:ILE:HG22	2.00	0.42
1:A:1005:HIS:CD2	1:A:1007:ILE:HB	2.55	0.42
1:A:1307:VAL:HG22	1:A:1338:THR:HG22	2.02	0.42
2:B:312:GLN:HE21	9:I:41:ASN:HD21	1.68	0.42
2:B:666:ASP:OD1	2:B:666:ASP:N	2.53	0.42
6:F:66:LEU:HD23	6:F:66:LEU:HA	1.87	0.42
1:A:513:ALA:HB2	6:F:90:LEU:HD21	2.02	0.41
4:D:76:ASN:OD1	4:D:77:ARG:N	2.53	0.41
9:I:12:VAL:HG13	9:I:13:GLY:N	2.34	0.41
17:Z:472:PHE:CE1	17:Z:520:LEU:HB2	2.53	0.41
1:A:551:ARG:HH12	8:H:27:ARG:NH2	2.16	0.41
1:A:757:GLN:NE2	1:A:778:LYS:O	2.54	0.41
2:B:422:PHE:CE2	2:B:429:PHE:HA	2.54	0.41
2:B:792:ASP:OD1	2:B:975:ARG:NH2	2.53	0.41
7:G:52:ASP:OD2	7:G:73:LYS:HE2	2.20	0.41
11:K:41:THR:O	11:K:45:ILE:HG13	2.20	0.41
11:K:45:ILE:HG21	11:K:45:ILE:HD13	1.83	0.41
1:A:916:PHE:CE1	1:A:963:ARG:HD2	2.55	0.41
2:B:83:ARG:HB2	2:B:133:ILE:HB	2.01	0.41
2:B:200:MET:HB2	13:N:24:DG:N1	2.35	0.41
2:B:252:ILE:O	2:B:303:PRO:HB3	2.20	0.41
2:B:692:THR:O	2:B:693:TYR:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:41:LYS:HE2	7:G:42:TYR:CZ	2.55	0.41
7:G:54:ILE:HD13	7:G:54:ILE:HA	1.88	0.41
1:A:120:ASP:OD1	1:A:121:SER:N	2.53	0.41
1:A:380:VAL:HG11	1:A:450:MET:HE3	2.02	0.41
1:A:902:GLU:O	1:A:978:VAL:HA	2.20	0.41
2:B:156:LEU:HD22	2:B:184:TYR:CZ	2.56	0.41
2:B:535:GLY:HA3	2:B:618:ALA:HB2	2.02	0.41
4:D:128:GLN:HE21	4:D:132:ASP:CG	2.28	0.41
1:A:563:LEU:HD23	1:A:563:LEU:HA	1.82	0.41
2:B:235:ILE:HG21	2:B:348:LEU:CD1	2.50	0.41
2:B:623:ARG:NH1	2:B:625:LEU:HD21	2.36	0.41
2:B:626:LEU:HD23	2:B:662:VAL:HG12	2.02	0.41
2:B:1062:ARG:HH12	2:B:1066:PRO:HD2	1.85	0.41
5:E:8:TYR:CE2	5:E:12:LYS:HE3	2.56	0.41
16:Y:60:ILE:HD11	17:Z:190:ARG:HG3	2.02	0.41
1:A:330:GLN:HG2	1:A:334:ARG:O	2.20	0.41
1:A:931:ARG:HD3	1:A:939:VAL:HG11	2.03	0.41
1:A:1474:LEU:HD11	6:F:107:ARG:NE	2.35	0.41
4:D:74:PHE:HB2	4:D:80:ILE:HG12	2.02	0.41
1:A:546:ARG:HG3	1:A:639:ILE:HG21	2.03	0.41
1:A:567:LEU:HD21	1:A:595:ILE:HG12	2.03	0.41
1:A:932:ARG:HG2	8:H:105:SER:O	2.21	0.41
1:A:1261:ILE:HG22	1:A:1262:MET:N	2.35	0.41
2:B:196:ALA:HA	2:B:394:ASP:O	2.21	0.41
2:B:817:GLN:HE21	2:B:912:ASN:ND2	2.18	0.41
3:C:75:SER:HB3	3:C:79:VAL:CG2	2.50	0.41
3:C:197:TYR:HD2	3:C:217:GLN:NE2	2.18	0.41
5:E:87:ILE:HD11	5:E:110:MET:CE	2.51	0.41
14:P:41:A:H2'	14:P:42:A:O4'	2.21	0.41
1:A:529:GLN:HG3	1:A:1094:SER:HB3	2.01	0.41
1:A:689:ILE:HD12	2:B:985:LEU:HD22	2.03	0.41
1:A:1155:LYS:HA	1:A:1309:MET:HE1	2.02	0.41
2:B:130:LYS:O	2:B:141:GLN:HA	2.20	0.41
2:B:154:ILE:HG22	2:B:155:MET:O	2.20	0.41
2:B:1124:ILE:HG22	2:B:1125:MET:H	1.86	0.41
1:A:88:ILE:HD12	1:A:253:LEU:HD23	2.03	0.41
1:A:375:ILE:HD11	1:A:669:TYR:HB2	2.02	0.41
1:A:406:VAL:HG21	1:A:440:LEU:HD11	2.02	0.41
1:A:1160:ARG:O	1:A:1300:GLY:HA2	2.21	0.41
2:B:25:ALA:HB1	2:B:640:ILE:HD13	2.02	0.41
2:B:46:SER:OG	2:B:397:GLY:N	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:721:ARG:HD3	2:B:721:ARG:HA	1.79	0.41
2:B:725:GLN:HG2	2:B:938:ARG:O	2.20	0.41
2:B:1104:ARG:HG3	2:B:1105:GLU:N	2.36	0.41
13:N:10:DA:C2	15:T:35:DA:C2	3.08	0.41
14:P:37:C:P	17:Z:579:LYS:HZ2	2.36	0.41
1:A:1130:ILE:HG21	1:A:1411:LEU:HD13	2.02	0.41
8:H:65:TYR:CE1	8:H:84:ARG:HB3	2.56	0.41
12:L:38:GLU:O	12:L:38:GLU:HG2	2.21	0.41
1:A:601:ASN:CB	1:A:988:TRP:CZ3	3.03	0.40
1:A:894:ASP:O	1:A:1022:ILE:HD13	2.21	0.40
1:A:1180:ASN:OD1	1:A:1183:SER:HB3	2.21	0.40
1:A:1197:TYR:O	1:A:1200:PRO:HD3	2.21	0.40
8:H:8:ASP:OD1	8:H:9:ILE:N	2.48	0.40
13:N:12:DT:H5"	17:Z:283:ARG:HH21	1.85	0.40
1:A:32:LYS:HE3	1:A:252:VAL:HG21	2.02	0.40
1:A:75:ALA:CB	2:B:1131:ARG:HD2	2.52	0.40
1:A:546:ARG:HD2	1:A:772:SER:HB3	2.04	0.40
1:A:601:ASN:HB3	1:A:988:TRP:CZ3	2.57	0.40
1:A:983:LEU:HD12	1:A:1044:HIS:CD2	2.57	0.40
2:B:67:LEU:O	2:B:84:TYR:N	2.39	0.40
2:B:88:PHE:CE2	2:B:412:LEU:HD21	2.56	0.40
2:B:674:MET:HB3	2:B:674:MET:HE3	1.89	0.40
2:B:771:GLU:O	10:J:55:LEU:HD21	2.20	0.40
2:B:830:GLU:OE2	2:B:870:THR:OG1	2.31	0.40
2:B:1051:LEU:HD23	2:B:1051:LEU:HA	1.77	0.40
3:C:26:THR:HG22	3:C:27:ASP:N	2.37	0.40
4:D:130:ILE:O	4:D:134:ILE:HG13	2.21	0.40
8:H:96:VAL:HB	8:H:116:VAL:HG22	2.03	0.40
9:I:120:GLY:O	9:I:122:ARG:HG3	2.22	0.40
1:A:77:ASN:C	1:A:79:THR:H	2.29	0.40
2:B:124:LEU:HD22	2:B:152:ILE:HD11	2.03	0.40
2:B:646:ARG:HG3	2:B:651:TYR:O	2.22	0.40
7:G:151:ARG:HH22	17:Z:477:HIS:HD2	1.68	0.40
1:A:425:ASP:CB	17:Z:583:PHE:CE1	3.05	0.40
1:A:536:GLY:O	1:A:538:VAL:HG23	2.22	0.40
2:B:248:LYS:O	2:B:252:ILE:HG12	2.21	0.40
2:B:260:LEU:HB2	2:B:263:ILE:HD12	2.03	0.40
2:B:853:LEU:O	12:L:46:LYS:NZ	2.55	0.40
4:D:38:HIS:CE1	4:D:69:ALA:HB2	2.56	0.40
5:E:185:ILE:CG2	5:E:209:VAL:HG21	2.47	0.40
17:Z:306:LYS:HA	17:Z:372:LEU:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:GLY:O	1:A:255:VAL:N	2.48	0.40
1:A:370:ASP:OD2	11:K:65:HIS:NE2	2.55	0.40
1:A:555:LEU:HD21	1:A:679:TRP:HE1	1.87	0.40
1:A:763:TYR:OH	8:H:23:ASP:OD2	2.18	0.40
1:A:1210:TRP:CZ3	1:A:1282:ASP:HB3	2.57	0.40
2:B:282:ARG:O	2:B:286:GLU:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1411/1970 (72%)	1353 (96%)	57 (4%)	1 (0%)	48	78
2	B	1143/1174 (97%)	1088 (95%)	55 (5%)	0	100	100
3	C	255/275 (93%)	238 (93%)	17 (7%)	0	100	100
4	D	126/142 (89%)	113 (90%)	12 (10%)	1 (1%)	16	48
5	E	207/210 (99%)	197 (95%)	10 (5%)	0	100	100
6	F	80/127 (63%)	78 (98%)	2 (2%)	0	100	100
7	G	169/172 (98%)	162 (96%)	3 (2%)	4 (2%)	4	29
8	H	146/150 (97%)	140 (96%)	6 (4%)	0	100	100
9	I	115/125 (92%)	105 (91%)	9 (8%)	1 (1%)	14	45
10	J	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
11	K	113/117 (97%)	113 (100%)	0	0	100	100
12	L	43/58 (74%)	40 (93%)	3 (7%)	0	100	100
16	Y	114/117 (97%)	113 (99%)	1 (1%)	0	100	100
17	Z	480/1087 (44%)	463 (96%)	13 (3%)	4 (1%)	16	48
All	All	4467/5791 (77%)	4265 (96%)	191 (4%)	11 (0%)	44	72

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	18	PHE
7	G	124	ASN
4	D	91	LYS
9	I	12	VAL
17	Z	362	GLU
7	G	155	ASN
17	Z	387	LYS
17	Z	497	GLU
1	A	529	GLN
7	G	20	PRO
17	Z	386	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1252/1749 (72%)	1252 (100%)	0	100	100
2	B	996/1027 (97%)	995 (100%)	1 (0%)	88	88
3	C	236/252 (94%)	236 (100%)	0	100	100
4	D	107/127 (84%)	105 (98%)	2 (2%)	50	65
5	E	189/190 (100%)	189 (100%)	0	100	100
6	F	71/111 (64%)	71 (100%)	0	100	100
7	G	149/153 (97%)	142 (95%)	7 (5%)	23	48
8	H	129/131 (98%)	128 (99%)	1 (1%)	73	76
9	I	105/112 (94%)	104 (99%)	1 (1%)	68	74
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	42/55 (76%)	42 (100%)	0	100	100
16	Y	102/103 (99%)	101 (99%)	1 (1%)	68	74
17	Z	429/940 (46%)	429 (100%)	0	100	100
All	All	3967/5112 (78%)	3954 (100%)	13 (0%)	84	83

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	187	ILE
4	D	68	THR
4	D	131	LEU
7	G	11	ILE
7	G	26	VAL
7	G	34	VAL
7	G	49	THR
7	G	66	VAL
7	G	97	LEU
7	G	163	LEU
8	H	96	VAL
9	I	95	VAL
16	Y	37	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	HIS
1	A	301	HIS
1	A	353	ASN
1	A	372	ASN
1	A	439	HIS
1	A	461	GLN
1	A	472	HIS
1	A	576	GLN
1	A	620	HIS
1	A	757	GLN
1	A	780	ASN
1	A	790	GLN
1	A	791	GLN
1	A	839	HIS
1	A	1032	GLN
1	A	1082	HIS
1	A	1163	HIS
1	A	1190	GLN
1	A	1360	ASN
1	A	1397	HIS
1	A	1417	HIS
1	A	1420	ASN
1	A	1457	ASN
1	A	1462	GLN

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Mol	Chain	Res	Type
2	B	111	ASN
2	B	265	GLN
2	B	312	GLN
2	B	350	HIS
2	B	370	HIS
2	B	460	HIS
2	B	471	ASN
2	B	518	HIS
2	B	639	HIS
2	B	731	GLN
2	B	817	GLN
2	B	825	GLN
2	B	986	GLN
2	B	1009	GLN
2	B	1021	HIS
2	B	1053	HIS
2	B	1097	HIS
2	B	1142	ASN
3	C	32	ASN
3	C	66	HIS
4	D	34	ASN
4	D	38	HIS
4	D	48	ASN
4	D	66	ASN
5	E	64	HIS
5	E	107	GLN
9	I	41	ASN
9	I	45	GLN
10	J	52	HIS
11	K	49	GLN
11	K	69	HIS
16	Y	12	HIS
16	Y	75	GLN
17	Z	234	HIS
17	Z	477	HIS
17	Z	509	HIS
17	Z	519	GLN
17	Z	534	HIS
17	Z	591	GLN
17	Z	595	HIS
17	Z	625	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	19/50 (38%)	4 (21%)	1 (5%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	35	U
14	P	36	A
14	P	37	C
14	P	41	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
14	P	36	A

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	14:DT	O3'	15:DT	P	3.16

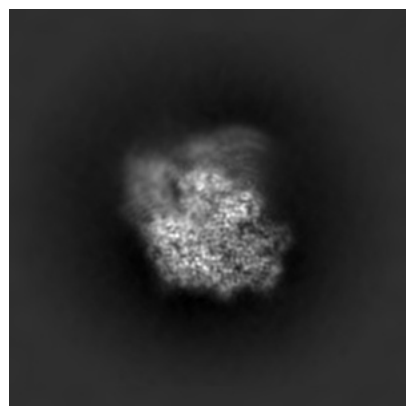
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3817. These allow visual inspection of the internal detail of the map and identification of artifacts.

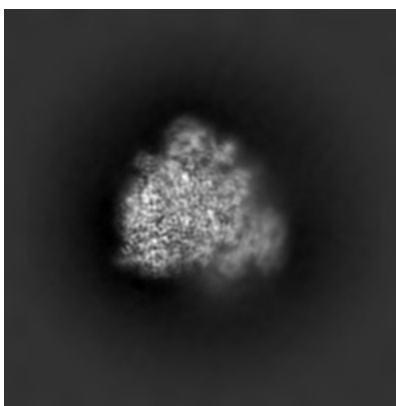
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

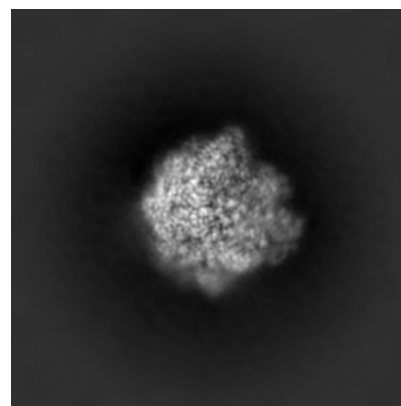
6.1.1 Primary map



X

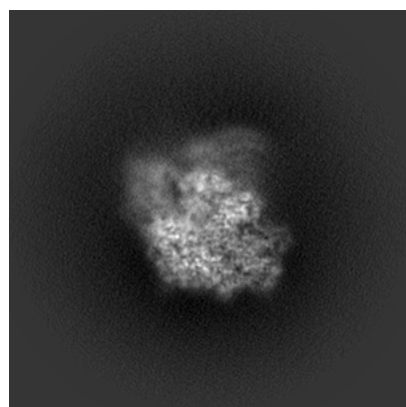


Y

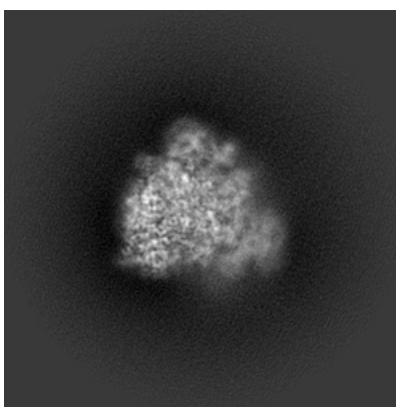


Z

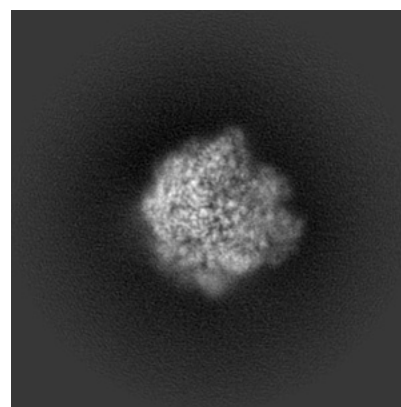
6.1.2 Raw map



X



Y

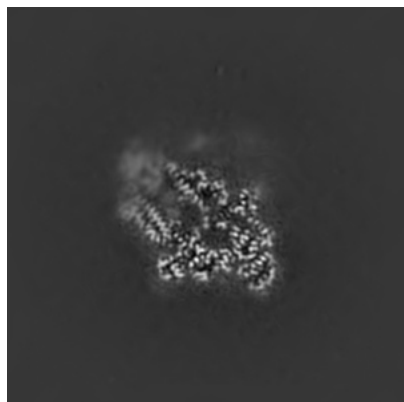


Z

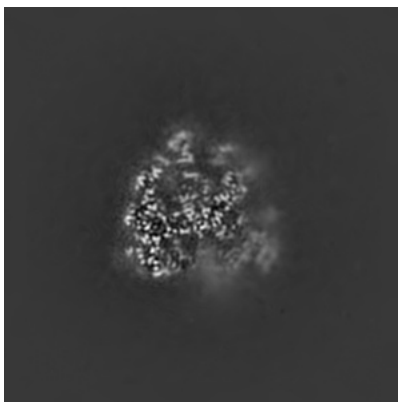
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

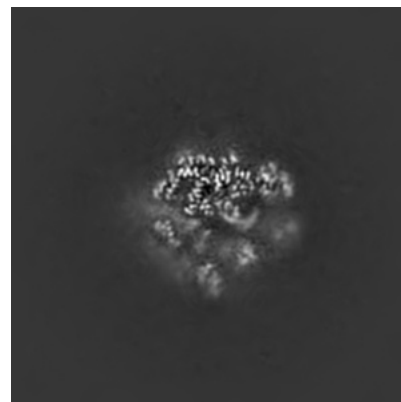
6.2.1 Primary map



X Index: 128

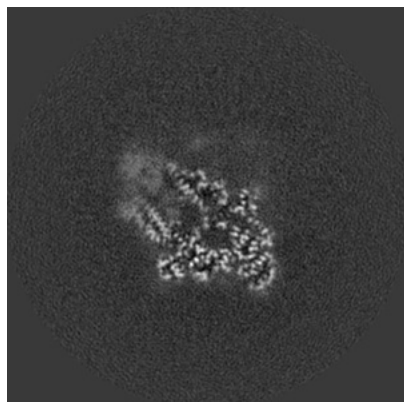


Y Index: 128

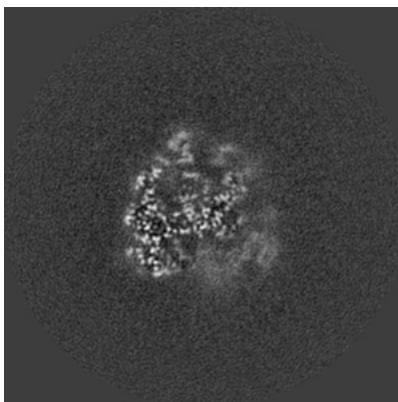


Z Index: 128

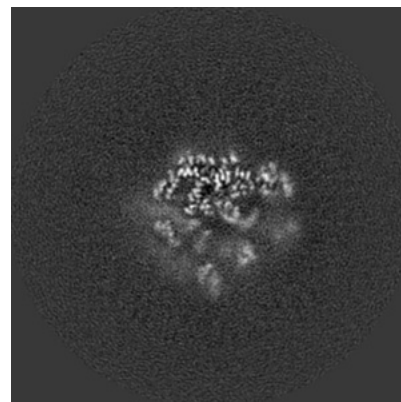
6.2.2 Raw map



X Index: 128



Y Index: 128

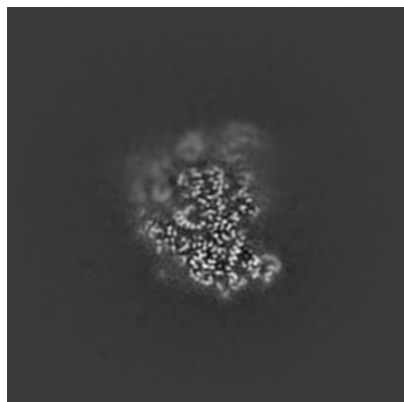


Z Index: 128

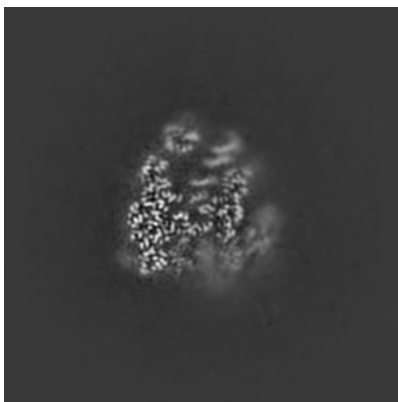
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

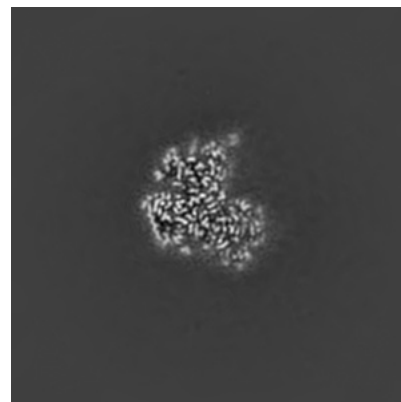
6.3.1 Primary map



X Index: 117

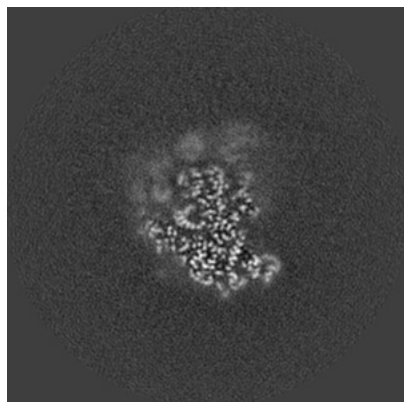


Y Index: 124

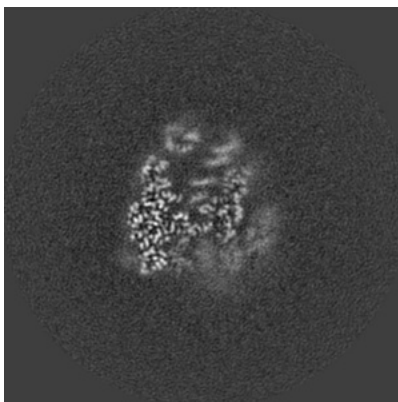


Z Index: 96

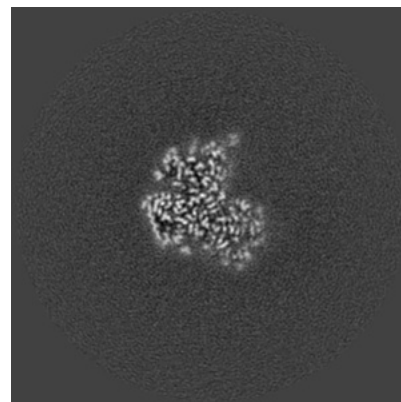
6.3.2 Raw map



X Index: 117



Y Index: 124

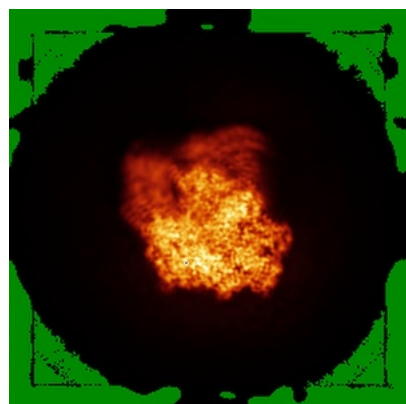


Z Index: 96

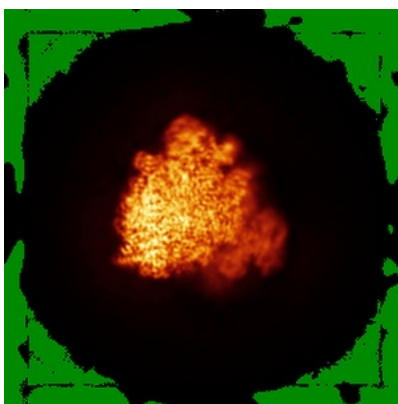
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

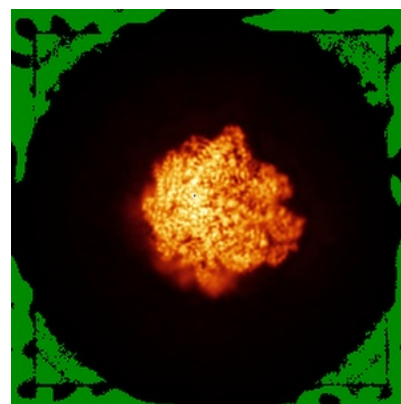
6.4.1 Primary map



X

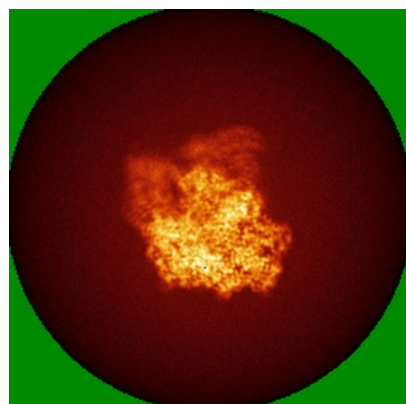


Y

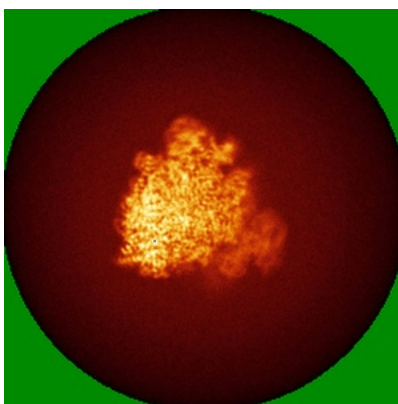


Z

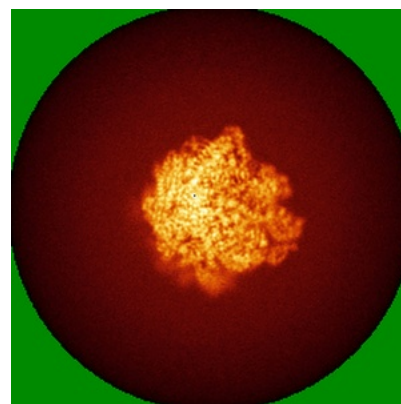
6.4.2 Raw map



X



Y

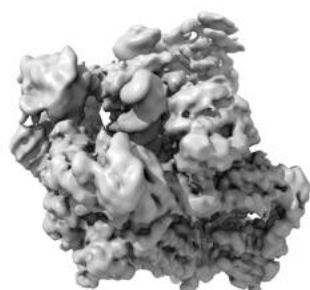


Z

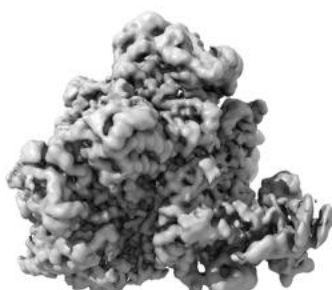
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

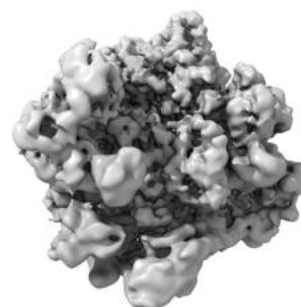
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

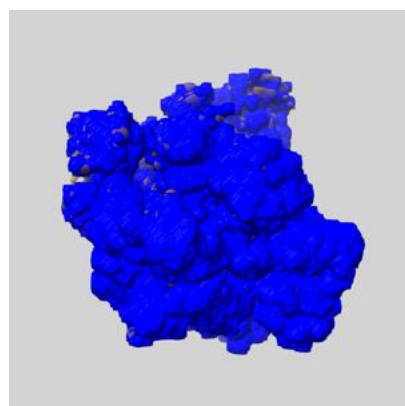
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

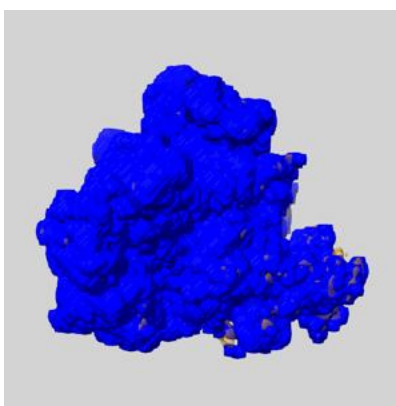
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

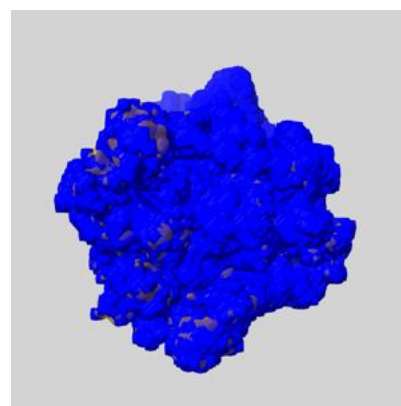
6.6.1 emd_3817_msk_1.map [i](#)



X



Y

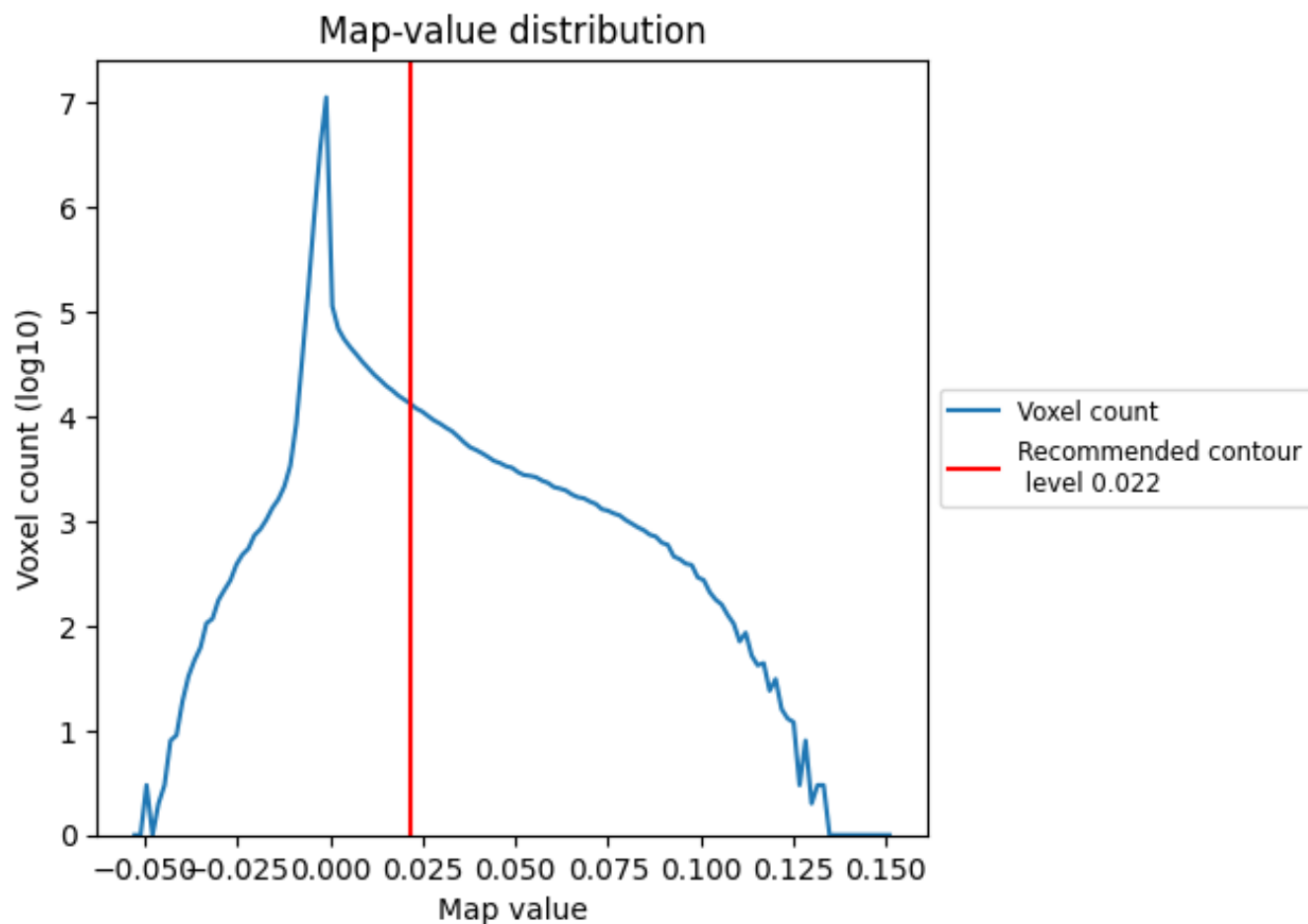


Z

7 Map analysis [i](#)

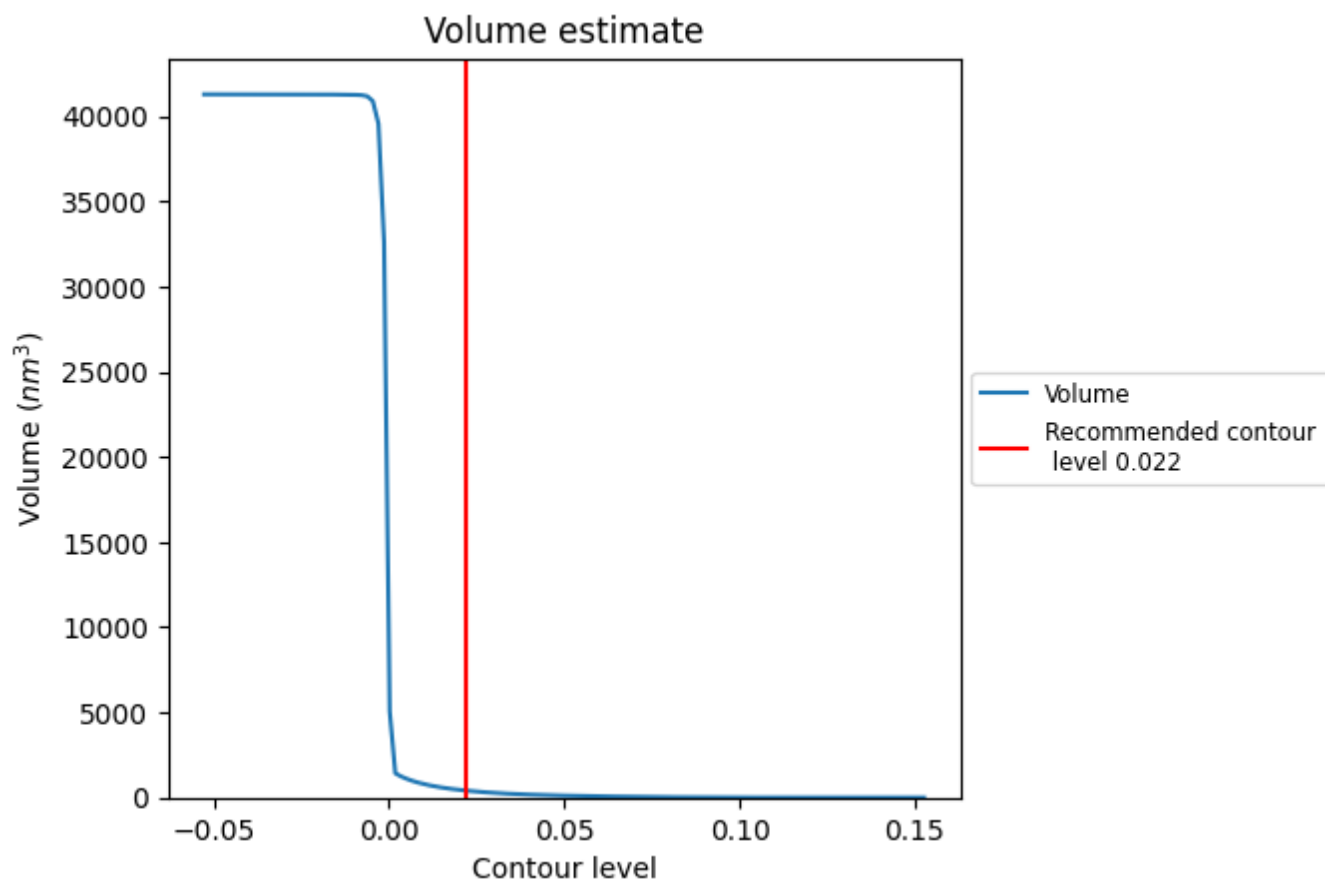
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

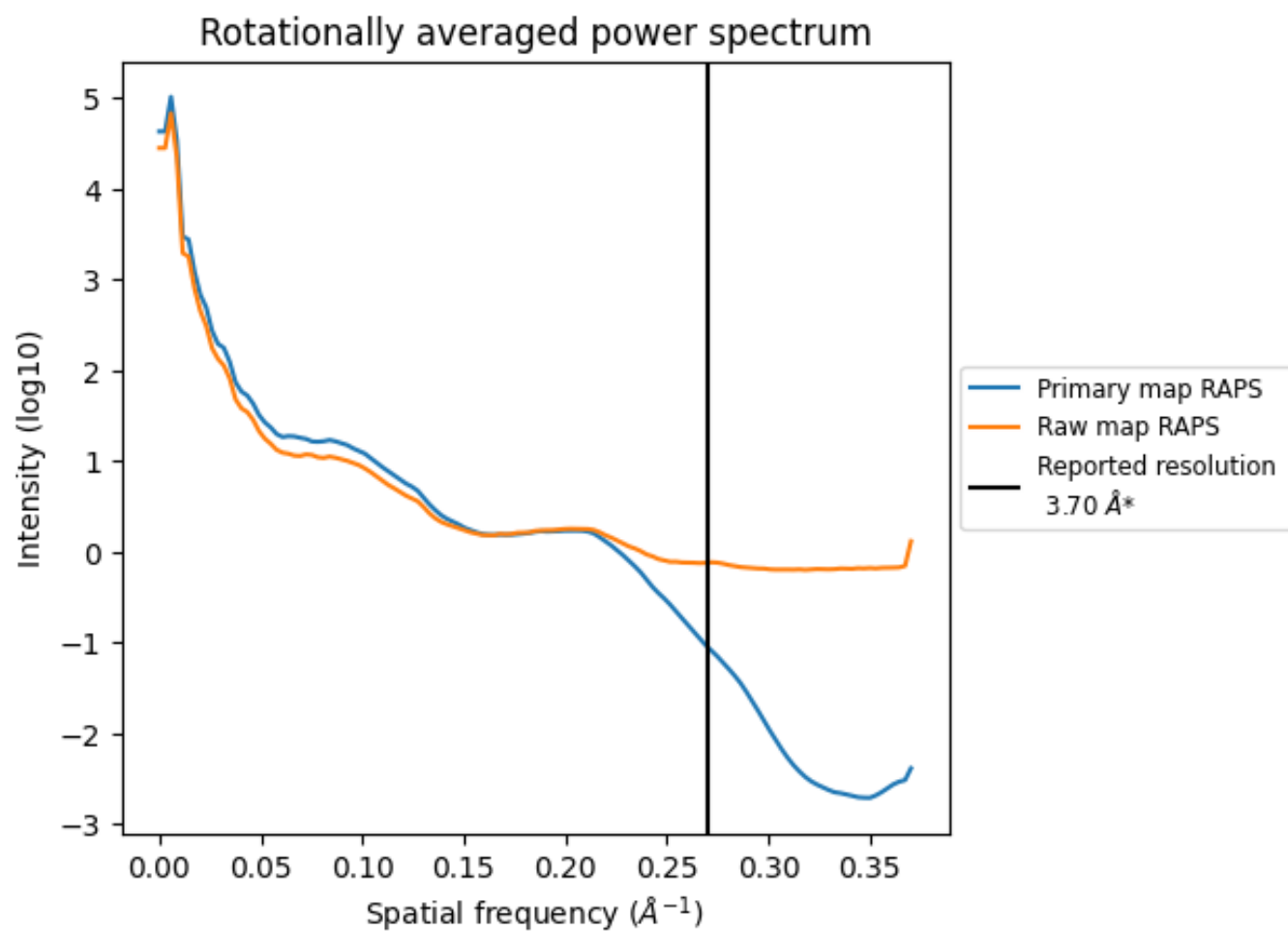
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 409 nm^3 ; this corresponds to an approximate mass of 370 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

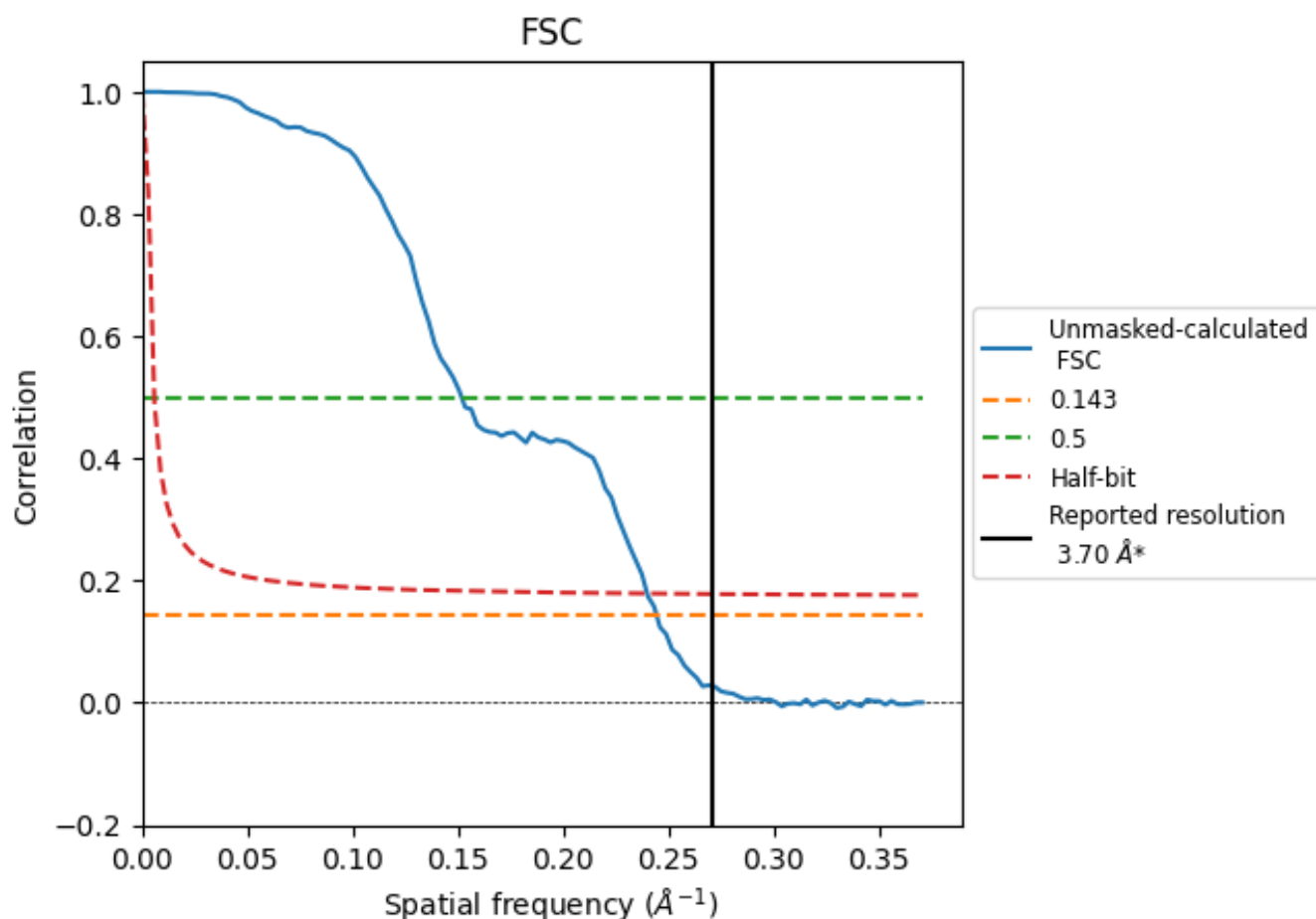


*Reported resolution corresponds to spatial frequency of $0.270 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.09	6.60	4.17

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.09 differs from the reported value 3.7 by more than 10 %

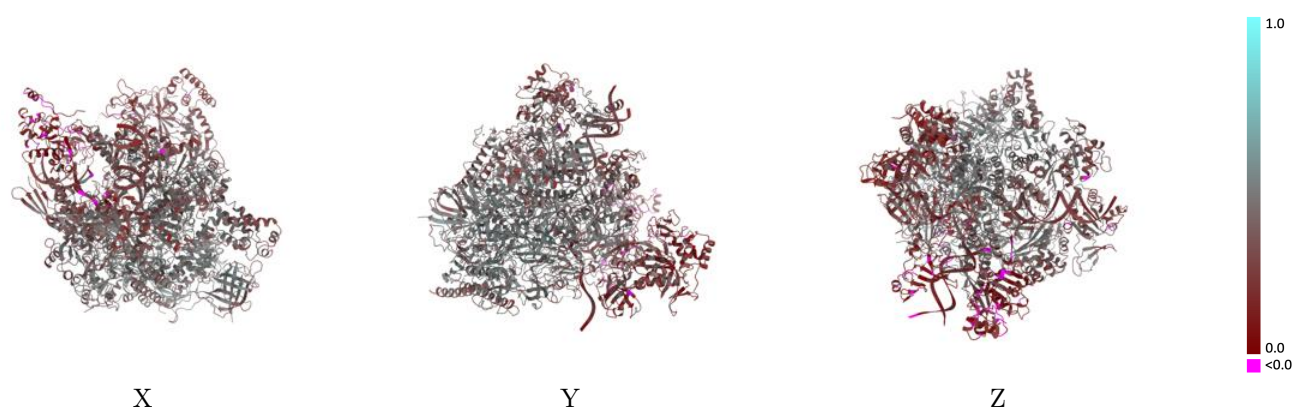
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3817 and PDB model 5OIK. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

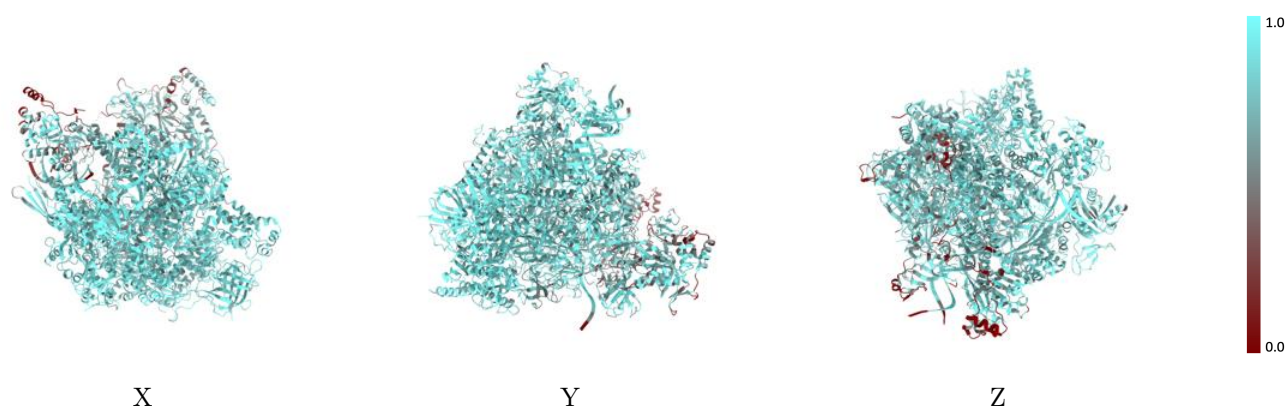
This section was not generated.

9.2 Q-score mapped to coordinate model [i](#)



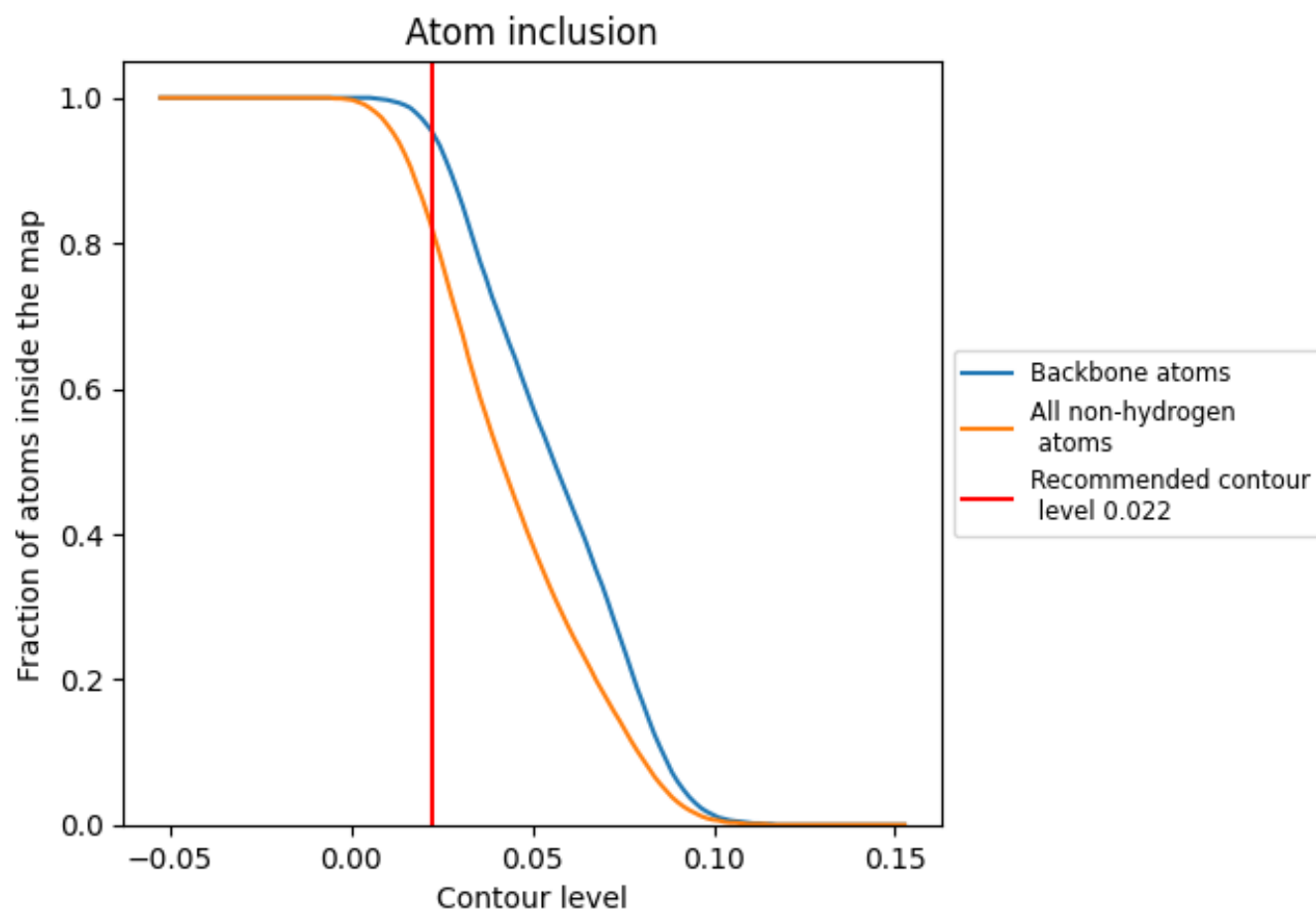
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8240	 0.3730
A	 0.8570	 0.4130
B	 0.8670	 0.4300
C	 0.9080	 0.4500
D	 0.5690	 0.2090
E	 0.8860	 0.3890
F	 0.8510	 0.4310
G	 0.7090	 0.2920
H	 0.8860	 0.4230
I	 0.8730	 0.3670
J	 0.8830	 0.4490
K	 0.8980	 0.4390
L	 0.8900	 0.4150
N	 0.8390	 0.2270
P	 0.8620	 0.3150
T	 0.8550	 0.2910
Y	 0.5350	 0.1090
Z	 0.6510	 0.2050

